Table 6. Enthalpy of formation, $\Delta_f H_{298}$ and $\Delta_f H_0$, heat capacity and entropy at 298 K, and H_{298}-H_0 from the original calculations. ***November 30 2006.***

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
Air (standard mixture)	28.96518	-0.126	-0.125		29.104	198.824	8.649	†
AL(cr) REFERENCE ELEMENT	26.98154	0	0		24.2	28.3	4.540	*‡
AL	26.98154	329.7		±4.2	21.391	164.555	6.919	†
ALH	27.98948	259.4		±20	29.348	187.857		*†
ALO	42.98094	66.944		±8	30.874	218.385		*†
ALOH	43.98888	-179.92		±13	31.877	216.419		*†
ALO2	58.98034	-86.192		±32	49.893	251.834		*†
ALO2H	59.98828	-460.247		±63	50.197	254.389		*†
AL2O	69.96248	-145.186		±17	52.035	252.336		*†
AL2O2	85.96188	-394.554		±32	67.192	280.996		*†
AL2O3(S)	101.96128	-1675.709			79.075	50.972		*†
AL2O3(G)	101.96128	-546.891	-544.39		86.990	316.662		†
AR REFERENCE ELEMENT	39.948	0	0		20.786	154.847	6.197	*‡
Ar+	39.94745	1526.778	1520..6	±0.001	20.984	166.406	6.206	†
B	10.811	560		±12	20.797	153.438		
B(S) REFERENCE ELEMENT	10.81	0.001			11.521	5.899		*‡
BCL	46.2637	141.417			31.675	213.246		*
BCLF	65.2621	-313.792		±29	42.557	264.655		*
BCL2	81.7164	-79.493		±12.6	47.438	272.691		*
BCL3	117.1691	-402.945		±2.1	62.476	290.188		*
BF	29.8094	-115.896		±13.8	29.567	200.473		*
BF2	48.80781	-589.959		±13	40.558	247.161		*
BF3	67.80621	-1135.646		±1.7	50.492	254.367		*
BH	11.81894	442.657		±8.4	29.178	171.849		*
BHF2	49.81575	-733.858		±3.3	42.341	244.025		*
BH2	12.82688	200.83		±63	34.062	180.211		*
BH3	13.83482	106.689		±10	36.211	187.886		*
BO	26.8104	-0.001		±8	29.179	203.472		*
BOCL OBCl	62.2631	-316.298		±29	45.102	237.435		*
BOF OBF	45.8088	-602		±13	40.996	224.806		
BOF2 OBF2	64.80721	-836.817		±15	50.253	267.853		*
BO2	42.8098	-284.518		±8	43.293	229.817		*
B2	21.622	829.687		±33.5	31.595	202.076		
B2O	37.6214	96.234		±105	38.402	227.747		*
B2O2 (BO)2	53.6208	-456.037		±8.4	57.4	242.629		*
B2O3(L)	69.6182	-1253.249			61.795	78.83		*
B2O3	69.6202	-835.975		±4.2	66.969	283.799		*
B3O3CL3 (BOCl)3	186.7893	-1631.706		±8	131.737	382.418		*
B3O3F3 (BOF)3	137.42641	-2365.152		±4.2	115.13	342.475		*
B3O3H3 BOROXIN	83.45502	-1217.544		±42	87.833	291.912		
H3B3O6 BORIC ACID	131.45322	-2271.833		±13	137.613	347.631		*
BaO	153.32640	-117.95	-		32.898	235.460		†
Br	79.904	111.86	117.93	±0.06	20.789	175.017	6.167	†
BrCl	115.35670	14.789	22.233		35.011	240.049	9.407	†
DBr	81.918102	-37.036	-29.160		29.228	204.484	8.668	†
BrF	98.902403	-58.851	-51.200	± 1.0	32.959	228.988	9.021	†
BrF3	136.89921	-255.6	-244.81	± 3.0	67.354	295.775	14.712	†
BrF5	174.89602	-428.8	-413.65	± 2.0	101.335	323.253	19.175	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
BRO	95.9034	125.8	133.333	±2.4	34.17	232.921	9.061	#
BrO2 Br-O-O	111.9028	108	116.091	±40	48.873	288.83	12.851	#
BrO2 O-Br-O	111.9028	152	161.545	±25	45.364	271.112	11.395	#
BrO3	127.9022	221	233.180	±50	59.995	284.507	13.101	#
Br2 (L) REFERENCE ELEMENT	159.8080	0	0		75.680	152.210	24.520	†
Br2 gas	159.8080	30.91	45.705	±0.11	36.057	245.469	9.725	†
Br2O BrBrO	175.8074	168	183.722	±20	51.385	312.704	13.137	†#
Br2O Br-O-Br	175.8074	107.6	124.061	±3.5	50.168	290.823	12.399	†#
Br2Pb Br-Pb-Br	3 67.008	-103.9	-87.54		56.966	339.673	15.022	†
C(GR) REFERENCE ELEMENT	12.011	0	0		8.528	5.734	1.054	*‡
C	12.011	716.67	711.198	±0.45	20.839	158.102	6.536	†
C+	12.01045	1809.444	1797.65	±0.8	20.974	154.664	6.649	†
CBr	91.91470	495.85	500.2		32.370	230.888	8.946	#†
CBrClF2	165.36421	-435.	-423.8	±15	74.650	318.724	15.528	†
CBrF3 Freon 1301	148.90991	-650.59	-638.48	±1.97	69.270	297.695	14.444	†
CBr2	171.81870	343.51	356.89		49.273	288.706	12.192	#†
CBr2F2	209.81581	-380	-366.88	±15	77.000	325.413	16.280	†
CBr3	251.72270	232.212	254.030	±4.2	69.174	331.466	16.015	#†
CBr4	331.62670	119.20	148.90	±1.5	91.162	358.185	20.396	#
CCL	47.46340	432.611	428.860		32.268	224.556	9.395	†
CCLF	66.46180	25.846	25.0	±30.	42.962	259.150	10.902	†
COCLF	82.4615	-426.779		±33	52.402	277.019		*
CCLF2	85.460206	-275.	-272.96	±25.	55.172	287.353	12.432	†
CCLF3 FC-13	104.45861	-710.02	-704.93	±2.19	66.887	285.424	13.791	†
CLCN Cyanogen Chloride	61.47044	137.952			45.333	236.344		*
COCL Carbonyl Chloride	63.4631	-62.756		±42	45.103	265.974		*
CCL2	82.91670	231.7	230.5	±1.7	51.028	266.112	11.728	#
CCL2F	101.91450	-105.	-103.57	±20.	59.121	298.917	13.217	†
CCL2F2 FREON-12	120.91291	-490.8	-486.62		72.477	300.908	14.881	†
COCL2 PHOSGEN	98.9158	-219.5	−217.80		57.761	283.752	12.879	†
CCL3	118.3697	71.128	71.553	±2.5	63.500	303.100	14.400	†
CCL3F FC-11	137.36720	-283.700	-280.53		78.071	309.785	16.064	†
CCL3O	134.36850	-18.41	-16.48		83.245	322.749		#
CCL4 liquid	153.823	-127.792		±0.55				X
CCL4	153.823	-95.815			83.618	309.995		†
CD	14.0251	599.700	596.251		29.206	192.997	8.795	#
CD A $^4\Sigma^-$ (Excited state only)	14.02480	670.477	667.158		29.176	189.887	8.657	#
CDH3	17.0489	-78.469			36.395	200.027		*
CDO Formyl – D Radical	30.0245	40.945	40.0		35.920	228.610		#
CD2	16.0392	382.601			36.282	204.302		*
CD2O	32.0386	-114.903			38.048	225.057		*
CD3	18.0533	137.537			41.845	207.031		*
CD3NO2	64.05885	-61.789	-48.423		63.166	291.669	13.556	#
CD4 RRHO	20.0674	-89.022			40.479	198.995		*
CD4 * ANHARMONIC	20.0674	-89.022			40.519	199.003		*
CD4O CD3OD	36.06651	-217.670	-207.07		49.478	249.248	11.932	#
CF	31.009103	246.932	243.333	±0.7	30.056	213.034	9.065	†
CF+	31.008554	1131.292	1121.86	±0.92	29.642	201.509	8.697	†
FCN	45.01614	35.987		±16.7	42.359	225.416		*
COF	47.0088	-171.539		±63	38.943	248.48		*
CF2	50.007506	-191.26	-191.73	±1.35	38.915	240.831	10.351	†
CF2+	50.006958	917.03	910.37	±1.6	38.541	246.731	10.342	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
COF2	66.00721	-640	-636.92	±5.	47.365	258.971	11.134	†
CF3	69.00591	-467.4	-464.6	±1.97	49.642	264.521	11.491	†
CF3+	69.00536	411.627	408.179	±1.96	49.339	254.540	11.541	†
CF3I	195.91068	-589.11		±3.3	70.941	307.633		
CF3O Radical	85.005309	-630.696	-625.69	±8.	64.550	283.750	13.622	#
CF3OO RADICAL	101.00501	-627.349			79.392	315.015		
CF4 FC-14	88.00461	-933.4	-927.15	±0.53	61.052	261.459	12.730	†
CH	13.01864	595.8	592.5	±0.6	29.175	183.037	8.625	#
CH A $^4\Sigma^-$ (Excited state only)	13.01864	667.919	664.583		29.151	182.626	8.624	#
CHBr	92.92264	377.857	384.99	±2.	39.789	252.872	10.416	#
CHBrClF	137.37374	-230.000	-217.24	±15	62.869	304.928	13.787	#
CHBrF2 HBFC-22B1	130.91975	-425.46	-412.26	±1.07	58.767	295.230	13.170	†
CHBr2	172.82664	198.489	215.446		54.834	298.588	12.851	#
CHBr3 Bromoform	252.73064	54.266	80.419		71.026	330.864	15.915	#
CHCL	48.47189	297.10	296.78		37.787	235.062	10.200	†
CHCLF	67.4703	-83.681			50.466	280.878		†
CHCLF2 HCFC-22	86.46845	-490.72	-484.38	±2.28	55.851	280.895	12.362	†
CHCL2	83.92487	95.8	97.469		53.900	285.500	12.800	†
CHCL2F FC-21	102.9233	-284.934			61.077	293.204		†
CHCL2O CCl_2OH	99.92374	-94.977	-91.0		69.410	307.164		#
CHCL3 liquid Chloroform	119.3779	-133.784		±0.72				X
CHCL3 CHLOROFORM	119.3779	-102.928			65.5	295.666		†
CHCL3O CCl_3OH	135.37644	-275.977	-270.06.	±3.2	86.644	323.540		#
CHD2NO2	63.05268	-57.716	-44.135		60.806	289.264	13.290	#
CHD3	19.0612	-85.305			38.893	208.581		*
CHF RADICAL	32.01734	163.176			34.585	228.715		†
CHF2	51.01575	-254			45.279	258.506		†
CHF3 FLUOROFORM HFC-23	70.01385	-693.289	-686.34		51.139	259.375	11.573	†#
CHI3 IODOFORM	393.73205	210.874	218.799	±4.2	75.072	355.672	17.157	†
HCN anharmonic	27.02568	129.799	180.136	±0.38	35.857	201.824	9.235	†
HNC	27.02568	191.908	191.530	±0.69	40.271	205.511	10.001	†
HNCO Isocyanic acid	43.02478	-118.600	-115.60	±4.2	45.078	238.265	10.966	†
HOCN Cyanic acid	43.02478	-15.456	-12.76	±20.	46.047	241.244	11.268	#
HCNO Fulminic acid	43.02478	167.603	171.042	±12	48.395	225.025	10.623	#
HONC	43.02478	234.164	235.73	±17.	49.654	248.364	12.400	#
CHN2	41.03242	319.796		±23.4	48.059	248.503		
CH(NO2)3	151.03556	-13.389	+4.976		134.09	435.569	25.968	
CHO FORMYL RADICAL	29.01804	42.3	41.928	±0.3	34.680	224.28	10.000	#
CHO+	29.0178	833.059	--		36.015	203.32	--	*
COH	29.01804	218.10	217.72	±0.83	34.970	225.030	10.008	#
COOH equilibrium	45.01744	-181.32	-178.16	±2.30	43.610	251.736	10.813	†
HCOO* Formyloxyl Radical	45.01744	-129.7	-126.955	±12.6	41.965	254.941	11.223	#
HCS	45.08494	300.47			37.059	236.148		
CH2 Methylene Equilibrium	14.02658	391.2	390.7	±1.6	35.130	194.436	10.032	#
CH2 Methylene SINGLET	14.02658	428.8	428.3	±1.6	33.781	189.220	9.940	#
CH2 Methylene Triplet only	14.02658	391.2	390.7	±1.6	35.014	194.418	10.027	#
CH2BrCL HALON101	129.38358	-45		±15	52.726	287.29		
CH2Br2	173.83458	4.937	26.329	±2.	54.554	293.767	12.650	#
CH2CL	49.47979	116.875			43.201	243.375		*†
CH2CLF GC-31	68.4782	-264.432			47.038	264.307		†
CH2CL2	84.93198	-95.396	-88.547	±0.74	50.951	270.365	11.854	†
CH2DNO2	62.04652	-52.532	-38,81		58.983	286.942	13.098	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
CH2D2	18.0551	-81.769			37.51	207.911	10.151	*
CH2F	33.02528	-32			40.292	236.529		†
CH2F2 FC-32	52.02339	-452.709	-444.65	±1.0	42.869	246.347	10.693	†
H2CN RADICAL	28.03362	240.162			37.768	224.304		
HCNH trans	28.03362	298.738			38.072	229.017		
HCNH cis	28.03362	319.658			38.892	229.493		
H2NCO	44.03302	-23.305		±9.9	52.926	256.458		
CH2NO CH_2=N-O*	44.03302	173.427		±21	49.153	249.913		
H2CNO H_2C*N=O	44.03302	223.928		±8.4	42.388	244.644		
CH2NO2 NITRO-METHYL RAD	60.03242	152.465	161.86		58.862	288.218	13.143	#
CH2NO3 Methyl Nitrate Radical	76.03182	98.952	109.481		76.78	312.169	16.347	
CH2N2 CYANAMIDE	42.04036	135.888		±20	51.505	247.641		
H2CN2 HN=C=NH	42.04036	149.005		±15	50.223	247.113		
CH2N2 H_2C=N=N	42.04036	286.382		±25	51.144	240.982		
H2CN2 CY DIAZIRENE	42.04036	320.143		±20	41.383	236.962		
CH2(NO2)2	106.03796	-61.505	-43.674		86.352	358.098	17.721	
CH2O FORMALDEHYDE	30.02628	-108.58			35.388	218.764		
HCOOH FORMIC ACID	46.02568	-378.57			41.305	247.148		
H2CS	46.09288	114.683			38.196	236.949		
CH3	15.03452	146.7	150.0	±0.3	38.417	194.008	10.366	#
CH3+	15.03397	1101.792	1099.37	±0.097	34.749	186.827	9.983	#
CH3BR	94.93852	-36.443	-21.034	±2.	42.312	245.954	10.607	#
CH3CL	50.48722	-81.87	-73.94	±0.6	40.741	234.396	10.416	†
CH3F FC-41	34.032923	-239.55	-231.52	±2.65	37.504	222.826	10.135	†
CH3Hg Methyl Mercury	215.62452	188.28	200.21	±8.4	46.073	260.58	11.165	#
CH3I Methyl Iodide	141.93899	14.30	23.838	±1.4	44.084	253.007	10.816	†#
CH3N (H_2C=NH) Methanelmine	29.04126	84.015	91.93	±4.5	38.084	221.567	10.176	#
CH3N Methyl-N Radical	29.04126	319.950	327.711	±4.5	39.990	226.694	10.330	#
CH3NO NITROSOMETHYL	45.04096	79.002		±7.3	50.77	260.833		
OCHNH2 FORMAMIDE	45.04096	-195.263		±10.5	48.473	253.646		
CH2NOH	45.04096	29.288			53.359	248.547		
NCH3O FORMIMIDIC ACID	45.04096	-148.436		±10.9	43.477	254.079		
H3CNO CH_2-NH=O	45.04096	59.032		±11.5	44.542	250.67		
CH3NO2 NITRO-METHANE	61.04036	-80.751	-66.85		55.528	282.863	12.610	#
CH3NO2 Methyl Nitrite CH_3ONO	61.04036	-65.44	-54.015	±1.	64.891	302.910	15.345	#
CH3NO3 METHYL-NITRATE	77.03976	-122.005	-107.13	±4.2	76.597	305.793	16.234	
CH3N2 CH_3N=N*	43.0483	247.651		±12	53.694	257.186		
CH3N3 CH_3-N=N=N MethylAzide	57.05474	297.29	309.93	±8.	63.015	279.531	14.118	#
CH3O	31.03392	21.0	28.4	±2.1	42.541	234.278	10.719	#
CH2OH	31.03392	-17.0	-10.7	±0.7	47.401	244.170	11.781	†
CH2OH+	31.03337	716.400	718.149	±0.3	37.835	228.047	10.149	†
CH3OD	33.04832	-205.331	-194.49		44.142	242.751	11.543	#
CH3O2 Peroxymethyl Radical	47.034	9.0		±5.1	52.257	268.762		
CH3S Thiomethoxy Radical	47.10082	124.6		±1.7	46.64	242.040		#
CH4 RRHO	16.04276	-74.6	-66.633	±0.3	35.613	186.314	10.023	
CH4 ANHARMONIC	16.04276	-74.6	-66.626	±0.3	35.691	186.371	10.016	†
CH4N CH_3NH*	30.0492	187.569		±4.8	47.372	235.967		
CH4N *CH_2NH_2	30.0492	153.49	164.62	±8.	48.597	244.694		#
(NH2)2C=O Urea	60.05534	-231.999	-215.617	±8.	77.445	299.707	14.618	#
CH4N4O2 Nitroguanidine, Picrite	104.06822	89.295	113.750	±8.	106.201	358.208	19.555	
CH4N4O2 NG $(NH_2)_2C$=N-NO_2	104.06822	48.162	73.401	±8.	106.906	348.642	18.762	#
CH3OH(L)	32.04216	-238.91	-235.57		81.080	127.269	18.995	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
CH3OH	32.04216	-200.94	-190.11		44.039	239.81	11.444	#†
CH4O2 (CH_3OOH)	48.04126	-126.733	-114.22	±4.2	66.753	275.904	14.160	#
CH4S (CH_3SH)	48.10876	-22.525			50.415	258.382		
CH5N CH_3-NH_2	31.0574	-23.025			50.505	240.75		*
CH5N2 CH_3N*NH_2	45.06418	215.183		±5.5	63.575	260.107		
CH5N3 GUANIDINE	59.07062	27.952	48.939	±8.	75.796	297.900	14.223	#
CH6N2 MethylHydrazine	46.07182	109.41	130.443	±8.	68.911	274.188		#
CH6Sn CH_3SnH_3	136.76834	118.407	136.091	±4.2	73.750	285.712	15.907	#
CI3 Triiodomethyl Radical	392.72411	405.984	410.000	±60.	70.550	361.033	16.831	#
CI4 TetraIodoMethane	519.62858	260.41	265.53		95.819	391.347	22.327	#
CN	26.01774	438.68	435.4	±2	29.156	202.643		#
CNO (NCO)	42.01684	128.040	127.57	±4.2	39.989	232.229	10.198	†#
CNN	40.02418	591.87	591.216	±3.19.	42.656	232.398	10.378	†#
NCN (NCN)	40.02418	465.89	465.433	±1.78	41.946	225.814	10.180	†#
C(NO2)4 TetraNitroMethane	196.03316	82.383	101.856		176.119	503.723	33.993	
CO	28.0104	-110.53		±0.17	29.141	197.657		†
COS	60.0764	-138.399		±1	41.556	231.475		*†
CO2	44.0098	-393.51		±0.13	37.135	213.787		†
CP	42.984461	520.162	517.860	±10.	29.910	216.257	8.715	†
CS	44.0767	278.550	275.307	±3.8	29.799	210.559	8.708	†
CS2 Anharmonic	76.143	116.70	115.913	±1.	45.482	237.889	10.664	†
C2	24.0214	824.35	816.288	±1.6	43.549	197.097	10.169	†
C2Br	103.9260	623.667	626.39	±2.	45.103	295.017	11.648	#
C2Br2	183.8300	335.31	346.51	±2.	68.067	294.448	15.427	#
C2Br2F4 HALON 2402	259.82361	-790.776		±4.2	120.019	252.529		
C2Br3	263.7340	385.388	405.674		83.269	369.892	18.602	#
C2Br4	343.638	215.584	218.816		102.196	387.413	22.410	#
C2Br5	423.54200	283.257	318.915		126.162	444.694	27.749	#
C2Br6	503.44600	165.480	209.480		146.665	459.134	31.667	#
C2CL	59.4747	494.09			45.046	241.948		†
C2CL2	94.9274	226.6		±14	65.668	271.942		*†
C2CL2F2 CCLF=CFCL E(trans)	132.92361	-341.486	-339.3	±8.	87.333	327.192	17.925	#
C2CL2F2 CCLF=CCLF Z(cis)	132.92361	-339.548	-337.37	±8.	87.632	327.213	17.934	#
C2CL2F4 FC-114	170.92101	-900.4			116.6	364.2		
C2CL3	130.3801	190.28			76.033	328.166		†
CCl2F-CCLF2 FC-113	187.37531	-705.8			121	386.9		
C2CL3F3 FC-113A	187.37531	-740.6			120.3	369.3		
C2CL4	165.834	-24.2	-23.336	±8.0	94.92	340.925	19.606	†
C2CL5	201.2855	39			118.832	397.906		
C2CL6	236.7376	-162.110	-159.69	±8	136.326	407.696	27.235	†#
C2D2	28.0502	222.194	222.675		49.556	208.92		*
C2D2O	44.0496	39.932			55.669	249.614	12.388	*
C2D4	32.0784	30.279			52.064	230.672		*
C2OD4	48.0778	-180.582			64.697	275.315	14.042	*
C2D6	36.1066	-110.676			64.743	244.479	13.228	*
C2D6N2 Azomethane-D6	64.12001	119.248			92.1	312.346		*
C2D6O DimethylEther-D6	52.10601	-209.49	-192.04		77.528	283.259	15.875	*
C2F	43.019803	353.847	350.00	±50.	42.6	231.036	10.367	†
C2F2	62.018206	-144.666	-147.	±20	60.114	249.570	13.266	†
C2F3	81.01661	-228.175	-227.0	±20.	66.178	297.643	14.164	†
C2F4 FC-1114	100.01501	-675.34	-671.91	±2.0	80.459	300.128	16.331	†#
C2F5	119.01402	-891.192			94.111	341.49		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C2F6 FC-116	138.01182	-1347.38	-1339.0	±0.31	106.294	341.033	20.229	†#
CF3-O-O-CF3	170.01122	-1507.077		±12.5	137.807	433.17		
C2H ETHYNYL	25.02994	568.522		±4	41.999	213.304		†
C2HBr	104.93394	282.43	289.073	±2	55.087	252.719	11.948	#
C2HBr2	184.83794	333.590	348.909		68.272	326.691		#
C2HBr3	264.74194	144.13	168.884		85.590	359.979		#
C2HBr4 1,1,2,2-$CHBr_2CBr_2$	344.64534	218.823	250.685	±8.4	107.701	425.045	23.519	#
C2HBr4 1,1,1,2-CBr_3CHBr	344.64534	243.634	274.593	±8.4	113.967	417.090	24.422	#
C2HBr5	424.54994	113.09	153.50		126.586	439.181		#
C2HCL	60.48264	226.4		±10.	54.32	241.999		†
C2HCLF 1,1-CLF Radical	79.48074	101.87	103.90	±8.	63.592	289.422	13.317	#
C2HCLF2-1,1 FC-1122	98.478846	-333.654	-329.16		76.650	304.242	15.263	†
C2HCLF2 cis FC-1131	98.478846	-323.569			75.394	305.096		
C2HCLF2 trans	98.478846	-323.103			75.149	304.318		
CF2H-CCLF2 FC-124A	136.47625	-903.3			100.4	351.1		
CF3-CHCLF HCFC124	136.47625	-924.7			99.06	349.6		
C2HCL2F-1,1+cis+trans	114.93314	-168.648	-164.97		77.324	320.190	16.259	†
CF3-CHCL2 HCFC123	152.93055	-743.9			102.6	352.6		
CF2CL-CHFCL FC123A	152.93055	-710			104.5	368.1		
CFCL2-CHF2	152.93055	-702.1			104.5	361.7		
C2HCL3	131.38804	-17.5	-14.0	±3.0	80.016	324.941	16.605	†
C2HCL4	166.84014	21.824	26.108	±8.	100.608	375.159	20.419	#
C2HCL5	202.29284	-160.410	-153.83	±8.	113.348	379.920	22.716	#
C2HF	44.027743	41.692	41.	±25	52.268	231.573	11.446	†
C2HF2	63.02615	-42.5	-40.52	±17.9	59.249	279.393		#
C2HF3	82.02455	-490.78	-485.53	±8.24	69.191	292.665	14.328	†
C2HF5 FC-125	120.02136	-1120.00	-1110.4	±8.	95.808	334.635	18.776	#
HCCN	39.03668	610.431		±100	54.238	240.596		
C2HNO NC-CHO	55.03548	44.120	46.152	±8.	55.793	270.935		#
C2HNO2 HCC-NO_2	71.03488	278.654	283.597	±8.	69.580	289.604	14.414	#
HCCO Ketyl Radical	41.02934	177.402		±8.8	48.417	245.287		
H2C2 VINYLIDENE	26.03728	414.788	414.489		42.614	221.021	10.874	†
C2H2 ACETYLENE	26.03728	228.20	228.769	±0.8	44.001	200.917	10.006	†
C2H2Br2 1,2-DiBromoEthylene	185.84528	101.9	121.55	±8.	69.521	315.102	15.447	#
C2H2Br4 $CHBr_2CHBr_2$	345.6532	53.35	89.89		107.863	398.747		#
C2H2CL CHCL=CH* Radical	61.48998	274.767	277.937	±8	53.700	270.153	11.996	#
C2H2CLF	80.48868	-165.393	-159.0	±15	64.216	283.339		†
C2H2CL2 CCL_2=CH_2	96.94328	2.2	8.084	±1.4	67.722	288.285		#
C2H2CL3 CH2-CCL3	132.39538	82.81	88.908	±5.	94.764	329.695		#
C2H2F2-1,1+cis+trans equilib.	64.03409	-336.4	-329.48	±4.	60.237	266.054	12.480	†
C2H2F2-1,1 FC-1132A	64.03409	-336.4	-329.48	±4.	60.123	266.041	12.476	#
H2C2F2 *cis*	64.03409	-306.5	-299.80	±5.	58.349	268.723	12.701	#
F2C2H2 *trans* FC-1132	64.03409	-303.73	-297.15	±5.	60.074	267.847	12.955	#
C2F3H2	83.03309	-517.142			79.499	303.093		
CF3-CFH2	102.03089	-913.3	-902.01	±17.5	86.273	315.752	16.937	#
CHF2-CHF2 HFC-134	102.03089	-883.3	-872.21	±5.5	84.129	313.143	17.130	#
C2H2N CH2CN Methyl-Cyanide	40.04402	257.78	260.54		54.345	255.826	12.356	#
C2H2N CH2NC Methyl Isocyana	40.04402	358.23	360.59	±8.	53.971	256.71	12.550	#
C2H2NO NC-CH_2-O*	56.04342	175.619	181.426	±8.	61.512	281.028	13.444	#
C2H2NO2 NC-CH_2-O-O*	72.04282	177.987	185.371	±8.	74.150	312.514	16.207	#
1,2-C2H2(NO2)2 trans	118.04896	40.953	56.131	±8.	108.234	360.962	21.428	#
CH2CO Ketene	42.03728	-47.698		±1.7	51.744	241.896		†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
HCCOH ETHYNOL	42.03728	93.186		±18.3	57.403	249.142		
C2H2O2 trans & cis GLYOXAL	58.03608	-212.082	-206.51	±0.8	60.409	272.483	13.682	†
C2H2O2 CIS GLYOXAL	58.03668	-193.35		±0.8				X
C2H2O2 Oxyranone	58.03608	-177.916	-170.37	±8.	53.635	263.960	11.713	#
C2H2O4 Oxalic Acid	90.03488	- 731.8	-721.2	±2.0	86.149	320.662		#
C2H3 VINYL RADICAL	27.04522	296.580	300.867	±0.92	42.071	233.663	10.522	†#
C2H3+ Vinylium Ion	27.04467	1122.34	1119.2	±1.17	50.714	225.350	11.780	#
C2H3BrO2 Bromoacetic Acid	138.94802	-383.5	-364.61	±3.1	80.542	337.015		#
CH3CBr3 1,1,1-Tribromoethane	266.75722	-26.3	+5.258		97.982	355.210		#
C2H3CL	62.49792	37.872	45.452	±8.	53.681	264.024	11.820	#
C2H3CLO3	94.49672	-427.6	-416.0	±1.0	78.839	325.918		#
C2H3CL3 CH_3-CCL_3	133.40332	-144.6	-133.98	±2.0	92.410	320.413	18.025	#
C2H3F	46.043623	-140.1	-132.21	±2.5	50.407	252.674	11.336	#
C2H3F2	65.04263	-302.503			67.256	288.291		
CH3CF3 FC-143A	84.04043	-755.655	-742.91	±1.0	78.074	287.652	15.298	#
CH3CD3 1,1,1-Ethane-D3	33.087526	-107.57	-92.313	±3.3	57.385	241.997	12.406	#
C2H3I Ethyl-Iodide	153.94969	128.867	137.906		56.071	299.640	12.368	#
C2H3N CH_3CN Methylcyanide	41.05196	74.04	81.09	±0.37	52.249	243.267	12.094	#
C2H3N CH_3NC Methylcyanate	41.05196	163.5	169.982	±7.2	52.947	246.658	12.660	#
C2H3NO $NCCH_2OH$	57.05136	-49.910	-39.97	±8.	64.965	280.796		#
C2H3NO2 $NCCH_2$-O-OH	73.05136	29.476	39.641	±8.	82.503	323.081	17.659	#
C2H3NO2 Nitroethylene	73.05136	33.284	46.001	±8.6	73.68	300.503	15.108	
C2H3NO4 $CH_3C(O)$-O-NO_2	105.04956	-303.654	-287.915	±8.0	101.794	351.943	20.765	#
C2H3NO5 $CH_3C(O)$-OO-NO_2	121.04896	-254.642	-237.021	±8.0	116.800	373.968	23.223	#
C2H3O (CH_3CO) RADICAL	43.04462	-10.3	-3.6	±1.8	50.785	267.448	12.385	#
C2H3O+ (CH_3CO+) ion	43.044714	669.952	670.921	±0.85	52.589	243.392	11.977	#
C2H3O (CH_2=CHO*) Radical	43.04462	12.753	20.189	±8.	52.398	258.818	11.713	#
OH3C2 (*CH_2CHO) RADICAL	43.04462	25.102			54.974	267.919	12.910	*
C2H3O OXYRANE RADICAL	43.04462	164.473	172.900	±8.0	45.741	252.528	10.723	#
C2H4 ETHYLENE	28.0536	52.500	61.025		42.887	219.322	10.519	†
C2H4Br2 CH_2Br-CH_2Br	187.8611	-37.5	-10.491		75.948	329.088	16.422	#
C2H4Br2 CH_3-$CHBr_2$	187.8611	-41.	-13.725		79.452	327.355	16.288	#
C2H4CL RADICAL	63.50646	90.12			58.635	281.459		
C2H4CL2 CH_2CL-CH_2CL	98.95856	-130.069	-117.37	±0.6	72.544	303.542	15.531	#
C2H4CL2 CH_3-$CHCL_2$	98.95856	-127.6		±1.1				X
C2H4O2CL2 Cl_2-Peroxyethane	130.95796	-231.375	-215.17		109.993	362.046	20.697	#
C2H4F RADICAL	47.05216	-72.216			58.857	273.845		
C2H4F2 CH_2F-CH_2F HFC-152	66.04997	-447.55	-433.78		64.238	279.918		#
C2H4F2 CH_3-CHF_2 HFC-152a	66.04997	-497.0	-473.07	±8.0	87.266	282.502		#
C2H4O VINYL-ALCOHOL	44.05316	-124.683			61	289.996		
C2H4O OXYRANE	44.05316	-52.635	-40.082	±0.63	47.624	242.870	10.831	†
CH3CHO ACETALDEHYDE	44.05316	-166.19	-155.70		55.319	263.952	12.897	†
CH3COOH liquid Acetic Acid	60.0524	-484.216		±0.17				X
CH3COOH ACETIC ACID	60.0524	-432.253	-418.12		63.439	283.473	13.597	†
(HCOOH)2 Formic Acid dimer	92.0512	-820.951			96.177	332.671		*
C2H5 ETHYL RADICAL	29.06110	118.658	129.75	±2	50.484	247.118	12.185	†
C2H5Br BROMOETHANE	108.9651	-61.60	-39.65	±1.01	64.206	287.668	13.584	#†
C2H5CL CHLOROETHANE	64.5138	-106.827	-92.25	±0.41	62.738	276.274	13.294	#
C2H5CLO2 Chloroperoxyethane	96.5132	-212.966	-194.27		92.223	336.239	17.853	#
C2H5F FLUOROETHANE	48.0595	-275.21	-260.41	±4.9	59.575	270.530	12.888	#
C2H5I IODOETHANE	155.96557	-7.047	8.253	±0.56	71.670	298.362	14.575	#
C2H5NO2 NITROETHANE	75.06724	-103.784	-83.506	±5.	79.018	320.512	16.015	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C2H5ONO2 ETHYLNITRATE	91.06664	-154.975	-132.82	±8.	95.103	328.863	18.480	
C2H5N3 Ethyl Azide	71.081320	266.872	287.394	±8.	80.026	303.042	15.761	#
C2H5O* ETHOXY RADICAL	45.0609	-13.6	-0.2	±8.0	66.321	277.642	14.325	#
CH2CH2OH RADICAL	45.0609	-23.849	-11.640	±8.0	68.668	291.708	15.564	
CH3CH*OH RADICAL	45.0609	-54.030	-40.776	±8.0	64.038	288.991	14.263	#
C2H5O Dimethylether Radical	45.0609	0.960	14.079	±8.0	66.124	281.519		#
C2H5O2 EthylPeroxy Radical	61.06050	-28.70	-12.450	±8.4	73.721	299.991		#
C2H6 ETHANE	30.0694	-83.852	-68.232	±0.2	52.501	229.221	11.892	†
C2H6N $(CH_3)_2N$ Dimethylazide	44.07578	159.854	177.58	±8.	66.912	270.641.		#
C2H6N *CH_2-NH-CH_3	44.07578	156.58	174.07	±8.	70.233	279.671		#
C2H6N2 AZOMETHANE	58.0828	148.684			77.872	289.777		*
C2H6N2O2 $(CH_3)_2N$-NO_2	90.08192	-4.8	20.279		103.204	328.138	19.783	#
C2H5OH(L) ETHANOL LIQUID	46.06904	-277.51	-269.74		112.250	160.100	24.082	†
C2H5OH ETHANOL	46.06904	-234.95			65.309	280.593		†
CH3OCH3 DIMETHYLETHER	46.06904	-184.054			65.823	267.381		
C2H6O2 PEROXYETHANE	62.06844	-173.636			82.969	314.534		
CH3OOCH3 Dimethylperoxyde	62.0682	-125.5	-106.5	±5.0	80.717	308.409		#
C2H6S C_2H_5SH Ethanethiol	62.13564	-46.108			72.676	296.102		
C2H6S (CH_3SCH_3)Methylsulfide	62.13564	-37.53			74.099	285.851		
C2H6S2 CH_3-SS-CH_3	94.20164	-24.142			94.307	336.645		
C2H7N CH_3-NH-CH_3	45.08372	-15.259	+6.501	±8.	68.541	267.185		#
C2H7N2 $(CH_3)_2N$-NH*	59.09046	207.685	232.276	±8.	81.384	284.772		#
C2H8N2 SYM Dimethylhydrazine	60.099	94.491		±7.5	82.347	287.346		
C2H8N2 UDMH	60.099	53.22			91.524	302.186		
CCN	38.02814	679.07	674.474	±6.23	44.231	237.159	11.089	#†
CNC	38.02814	675.85	670.935	±5.89	45.042	233.804	11.357	#†
C2NO O=C*-CN	54.02754	210.00	207.188	±10.	56.145	278.187	13.594	#†
C2N2	52.03488	309.28	307.342	±1.03	57.085	242.204	12.715	†
C2N2O2Hg(s) Hg- Fulminate	284.6	386.						X
C2(NO2)2 Dinitroacetylene	116.03248	349.046	356.251	±8	102.603	353.895	20.933	#
C2(NO2)4 Tetranitroethylene	208.04356	N/A	N/A		184.031	468.771	35.016	#
C2(NO2)6 Hexanitroethane	300.05524	179		±5.9	273.376	667.098		
C2O	40.02080	291.039	287.000	±12.	43.134	233.624	10.486	†
C2S2	88.15340	376.660	373.831		62.030	274.120	13.760	†
C3	36.03210	839.949	831.0		42.202	237.613	12.109	†
C3D4	44.0894	262.675			64.125	254.286	12.650	*
C3D6	48.1176	32.885			72.411	251.394	13.152	*
C3F Radical	55.030503	564.957	559.052	±8	55.612	277.062	13.479	#
C3F3 FCC-CF_2*	93.02731	-134.419	-135.23	±8	81.990	326.463	17.210	#
C3F3 *CC-CF_3	93.02731	-79.078	-79.609	±8	80.749	313.306	16.929	#
C3F4 PerFluoroAllene	112.02571	-553.685	-551.89	±8	92.135	336.733	19.021	#
C3F6 Hexafluoropropene	150.02252	-1157.253	-1150.95	±8	121.759	373.675	23.337	#
C3F7 RADICAL	169.02182	-1347.122	-1339.5	±8	135.964	416.386	26.401	#
C3F8 FC-218	188.02023	-1760.121			147.248	406.145		
C3H HC≡C-C	37.04004	719.393	714.091	±8	53.430	247.795	12.696	#
C3HF7 FC-227EA	169.02092	-1564.816	-1552.4	±8	136.690	399.058	25.901	#
C3HN CyanoAcetylene	51.04678	368.414	367.225	±8	62.633	247.991	12.918	#
C3H2(1) CyPropenylidene	38.04888	476.976	477.960		44.222	236.204	10.645	
C3H2(3) H2C*-C≡C*	38.04888	651.030	650.361		54.719	254.549	12.298	
C3H2(3) *HC=C=CH*	38.04888	755.254	751.668	±62.7	67.953	260.782	15.215	
C3H2(1) HC-C≡CH*	38.04888	817.972	816.374	±62.7	58.770	251.691	13.227	
C3H2F3 CF_3-CH=CH*	95.04319	-376.895	-369.47	±8	90.727	323.105	17.442	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C3H2F3 CF_3-C*=CH_2	95.04319	-374.941	-367.82	±8	91.100	125.439	17.741	#
C3H2N HC*=CH-CN	52.05472	442.855	445.486	±8	59.531	272.030	13.333	#
C3H3 PROPARGYL RADICAL	39.05682	346—349		±8	64.891	256.659		†
CLC3H3 1-Chloro-1-propyne	74.50862	184.711	189.553	±8	71.364	283.822	15.611	#
C3H3Cl CH_2Cl-CCH	74.50952	162.729	167.78		73.747	296.899		
3-C3H3Cl CY	74.50952	218.333	225.43		66.257	281.203		
C3H3Cl CHCl=C=CH_2	74.50952	160.851	163.18		70.089	290.465		
C3H3F2 *CF_2-CH=CH_2	77.052726	-224.438	-216.93	±8	89.452	316.769		#
C3H3F3 CF_3-CH=CH_2	96.051130	-631.131	-619.51	±6.	90.704	319.468		#
C3H3I CH_2ICCH Propargyl Iod.	165.96039	269.072	276.353	±12.5	74.028	310.672	15.180	#
C3H3I CH_2=C=CHI Allenyl Iod.	165.96039	264.117	272.127	±12.5	70.463	305.857	14.451	#
C3H3N CH_2=CHCN	53.06266	184.037	190.874	±8	59.387	263.290	13.361	#
C3H3O CH_2=CHC*=O	55.05532	88.530	94.601	±8	61.410	300.654		#
C3H3O *CH_2-CH=C=O	55.05532	93.560	98.877	±8	68.927	293.760		#
H4C3 PROPYNE	40.06386	184.9	191.966		60.731	248.429	13.031	†
C3H4 ALLENE	40.06386	190.92	198.412		58.88	243.630	12.605	†
C3H4 CYCLOPROPENE	40.06386	277.1	285.823		52.883	243.605	11.374	†
C3H4CL *CH=CH-CH_2CL	75.51656	250.253	259.680	±8.	73.850	303.749	15.261	#
CLC3H4 *CH_2-CH=CHCL	75.51656	137.444	147.12	±8.	71.705	303.390	15.012	#
C3H4N CH_3-CH*-CN	54.07060	222.706	232.213	±8.	72.044	298.672	14.925	#
C3H4N2 1,3-DIAZOLE	68.07824	140.959		±28	65.701	273.426		
1,3,3 TRI-NITRO-AZETIDINE	192.08812	128.449	171.220	±8.	134.987	357.315	20.706	
C3H4O ACROLEIN	56.06416	-68.065	-57.913	±8	64.332	297.025		#
C3H4O2 CH_2=CH-C(O)-OH	72.06266	-326.051	-312.52	±8	79.301	313.570	15.243	#
C3H5 Symmetric Allyl Radical	41.0727	163.594			63.387	258.886		†
T-C3H5 CH_3C*=CH_2 “ “	41.0727	237.651			61.663	266.064		
S-C3H5 CH_3CH=CH* “ “	41.07180	265.533	276.287	±8.	63.362	271.305	13.577	#
C3H5 Cyclo	41.07180	279.91	292.716	±10.5	55.701	251.486		#
C3H5Cl 1-Chloro-1-propene	76.5245	-8.100	+4.937	±8.	76.450	299.193	15.884	#
C3H5CL 3-Chloro-1-propene	76.5245	0.369	14.052	±8.	74.210	307.919	15.239	#
C3H5N PROPIONITRILE	55.07944	53.191	66.974	±8.	72.039	285.205	14.883	#
CH3CH=CHNO2 Nitropropylene	87.07824	9.987	29.046	±8.9	93.59	330.004	18.288	
C3H5NO2 NitroCycloPropane	87.07824	21.033	41.466	±8.	90.786	311.278	16.913	#
C3H5N3O9 NITROGLYCERINE	227.08752	-279.073	-246.14	±2.7	234.24	545.865	43.458	
C2H5CO Propanal	57.0712	-32.83	-19.862	±8.	67.859	314.290		#
CH2COCH3 Acetone Radical	57.0712	-33.34	-20.617	± 8.	72.843	307.518		#
C3H5O Propylene Oxide Radical	57.0712	104.069	118.072	± 8.	71.197	293.196		#
C3H6 PROPYLENE	42.07974	20.000	35.014		64.433	266.668	13.551	†
C3H6 CYCLOPROPANE	42.07974	53.30	70.455		55.572	237.488	11.410	†
C3H6N2O2 N-NITRO-AZETIDIN	102.09292	114.123	141.198		100.656	328.954	18.840	
C3H6N6O6 RDX Solid	222.11748	79.078	--		284.884	146.189	--	
C3H6N6O6 RDX 135 Triazine	222.11748	192.000	233.285		230.174	482.441	39.331	
C2H5CHO Propionaldehyde	58.08004	-192.046			80.73	304.51		
CH3COCH3 ACETONE	58.08004	-214.814	-198.10	±0.26	74.207	295.660	16.193	†#
C3H6O PROPYLENE OXIDE	58.07914	-92.760	-74.271	±8.	72.671	281.487	14.415	#
C3H6O CY OXETANE	58.07914	-81.086	-61.49	±8.	61.826	274.672	13.499	#
C3H6O Vinylmethylether	58.07914	-100.378	-83.824	±8.	76.313	308.229	16.351	#
C3H6O Cyclopropanol	58.08004	-101.504	-81.907	±8.	70.158	277.454	13.308	#
C3H6S THIETHANE	74.14664	60.584			70.418	278.343		
N-C3H7 PROPYL RADICAL	43.0883	101.32	119.149	±1	71.309	290.460	14.970	†#
I-C3H7 ISOPROPYL RADICAL	43.0883	90.19	108.237	±2	65.545	290.109	14.725	†#
1-C3H7I Iodopropane	169.99305	-31.999		±2	85.883	332.737		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
2-C3H7I "	169.99305	-40.865		±2	91.193	334.082		
C3H5NH2 CY-PROPYLAMINE	57.09499	77.389			89.045	285.464	16.956	*
C3H7N AZETIDINE	57.09532	98.198			67.14	267.274		
C3H7NO2 Nitropropane	89.09412	-124.265	-97.795	±0.4	104.085	350.046	19.344	
C3H7NO3 NPN Propylnitrate	105.09262	-174.054	-146.91	±1.3	123.239	362.601	23.008	
C3H7NO3 L-Serine (gas)	105.09262	-579.107	-551.829	±8.	118.076	404.228	22.876	#
C3H7NO3 L-Serine (solid)	105.09262	-732.73		± 0.28		149.16		X
C3H7O N-PROPOXY RAD.	59.08798	-37.656			81.634	309.616		
C3H8 PROPANE	44.09562	-104.68	-82.388	±0.6	73.589	270.315	14.741	†
C3H7OH PROPANOL	60.09592	-255.2	-231.35		84.978	323.367	17.519	†
(CH3)2CHOH 2-Propanol	60.09592	-272.7	-248.59		89.594	309.226	17.265	†
C3H8O2 CH_3-O-CH_2-O-CH_3	76.0953	-346.967	-321.13	±8.	100.842	347.098		#
C3H8O3 (L) Glycerol (liq)	92.09382	-669.6		±0.6	218.9	37.87(s)		X
C3H8O3 Glycerol	92.09382	-577.9	-552.153	±1.1	131.648	400.000	24.306	
C3N2O NC-CO-CN	80.0449	247.5	246.523	±6.4	80.854	310.032	17.148	#
C3O2	68.0318	-93.64			67.37	276.816		†
C4	48.044	1033.904	1025.0		57.272	252.862	13.118	†
C4Cl2 Cl-CC-CCCl	118.94820	453.592	447.208	±8.	93.858	319.209	19.779	#
C4CL6 Perchloro-1,3-Butadiene	162.0343	-96.65	-97.33		38.364	110.307		
C4F2 FCC-CCF	86.03961	215.309	210.191	±8.	88.863	294.682	18.157	#
C4F6 Perfluoro 1,3-Butadiene	162.0343	-1004.122			137.272	388.442	24.949	*
F6C4 Perfluorocyclobutene	162.03439	-1210.843			131.589	379.256	25.135	*
C4F8 Perfluorocyclobutane	200.03123	-1513.6			145.483	405.3		
C4F10 FC-3110 Perfluorobutane	238.02803	-2137.417			189.038	480.624		
C4H	49.05194	803.328			66.759	265.569		
C4H2 Butadiyne	50.05988	458.299	456.653	±8	73.738	249.613	14.328	#†
C4H2N2 Fumaronitrile	78.072160	330.996	334.8	±8..	85.445	308.998	17.549	#
C4H3 E,1-butene-3-yne-1-yl	51.06662	543.104	545.65	±8	71.773	281.767	14.371	#
C4H3 i,1-butene-3-yne-2-yl	51.06662	501.829	502.00	±8..	77.383	305.368	16.739	#
C4H4 1-Butene 3-yne	52.07456	287.859	294.717	±8.	71.612	277.319	14.292	#
C4H4 Cyclobutadiene	52.07456	431.722	440.911	±8.	58.200	251.074	11.961	#†
C4H4N2 PYRAZINE	80.08804	195.811	212.069	±1.3	73.945	280.378	13.562	#
C4H4N2 PYRIMIDINE	80.08804	196.648	212.864	±1.	73.69	280.677	13.645	#
C4H4N2 SUCCINONITRILE	80.08804	209.7	221.172	±0.9	92.458	325.114	18.349	#
C4H4O FURAN	68.07516	-34.685			65.407	267.251		
C4H4O VINYL-KETENE	68.07516	22.719	31.98	±8.	81.797	309.171	16.229	#
C4H4O2 1,4-DIOXIN	84.07456	-86.0	-71.5	±7.	81.291	284.693		#
C4H4S Thiophene	84.14056	114.9	127.180		72.818	278.778	13.282	#
E-C4H5 1,3-butadiene 1-yl	53.08250	363.339	373.360	±8.	74.144	303.589	15.362	#
I-C4H5 1,3-butadiene-2-yl	53.08250	315.223	325.419	±8.	77.138	290.119	15.188	#
T-C4H5 1,2,butadiene-4-yl	53.08250	315.223	325.299	±8.	78.273	293.833	15.308	#
C4H5 1-butyne-3-yl	53.08250	318.432	327.890	±8.	81.537	293.840	15.926	#
C4H5 2-butyne-1-yl	53.08250	306.085	314.862	±8.	77.774	300.775	16.607	#
C4H5N PYRROLE	67.09044	108.18		±0.81	71.6	270.722		
C4H5N Cyclopropanecarbonitrile	67.09044	184.096		±0.84	78.734	321.389		
C4H6 1-Butayn Ethylacetylen	67.09044	165.2	178.798	±0.88	81.820	291210	16.020	†
C4H6 2-ButaynDimethylacetylen	54.09044	146.314	159.388	±8.	77.886	291.909	16.544	†#
1,3-C4H6 Butadiene	54.09044	110.834	125.118	±8.	74.219	293.330	15.335	†#
1,2-C4H6 Butadiene	54.09044	161.314	175.436	±2.	78.663	290.993	15.496	#
C4H6 Cyclobutene	54.09164	156.7	173.761		64.414	262.076	12.558	†
C4H6CL2 1,4-Dichlorobutene	124.99584	-51.882	-34.587	±8.	108.341	386.083	21.505	#
CL2C4H6 3,4-Dichlorobutene	124.99584	-53.572	-36.121	±8.	109.803	379.398	21.349	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C4H6O 2,5 Di-Hydro FURAN	70.08984	-108.78	-89.313		75.600	284.250	14.401	
C4H6O4 CH_3-CO-OO-CO-CH_3	118.08804	-500.	-477.02	±10	122.291	390.682	23.944	#
2,5 C4H6S Dihydrothiophene	86.15644	86.9	105.458		83.306	297.089	15.472	
C4H7 tt-1-Butene-1-yl	55.09838	245.871	262.755	±8.	83.705	311.281	16.968	#
C4H7 cc-1-Butene-1-yl	55.09838		264.85	±8.	-	-		X
C4H7 trans 1-Butene-2-yl	55.09838	231.162	248.45	±8.	83.973	300.371	16.425	#
C4H7 cis 1-Butne-2-yl	55.09838		248.11	±8.	-	-		X
C4H7 *trans*-2-Butene-2-yl	55.09838	223.853	239.743	±8.	83.237	313.256	17.962	#
C4H7 *cis*-2-Butene-2-yl	55.09838		243.09	±8.	-	-		X
C4H7 *trans* 3-Butene 1-yl Rad.	55.09838	204.595	220.915	±8.	84.719	317.348*	17.533	#
C4H7 cis 3-Butene-1-yl Radical	55.09838		223.01	±8.	-	-		X
C4H7 *trans* (CH2=CH*CHCH3)	55.09838	136.111	153.553	±8	80.787	306.087*	16.411	#
C4H7 *cis* –1-Methylallyl Radical	55.09838		156.48	±8.	-	-		X
C4H7 2-Methyl-Allyl Radical	55.09838	137.603	155.226	±5.	82.196	300.803	16.229	#
C4H7 Cyclobutyl Radical	55.09838	230.306	249.366	±8.	73.070	286.490	14.792	#
C4H7N C3H7CN Propylcyanide	69.10512	31.200	51.765	±8.	91.422	310.996	17.622	#
C4H7O 2-Butanone Radical	71.09778	-75.994	-57.670	±8.	97.420	344.655	19.868	#
C4H7O CH2=C(CH3)CH2O*	71.09778	55.748	75.378	±8.	96.143	334.259	18.562	#
C4H8 CH2=CH-CH2-CH3	56.107	-0.544			85.362	307.923	16.929	*
H8C4 CH2=C(CH3)2	56.107	-17.161			87.976	296.668	17.470	*†
C4H8 2-Butene trans	56.107	-10.975			81.112	300.751	17.023	*†
C4H8 2-Butene cis	56.107	-7.426			85.227	295.879	17.242	*†
C4H8 CYCLOBUTANE	56.10752	28.4			70.564	264.396		†
C4H8CL2S Mustard	159.07772	-124.77	-100.66		136.283	420.586	27.569	#
beta HMX solid	296.15664	74.894	--		307.302	145.101	--	
C4H8N8O8 HMX	296.15664	187.862	245.304	±25.1	275.455	568.833	50.045	
C4H8O 2-Methyl-Allyl Alcohol	72.10572	-161.143	-137.34	±2	100.007	316.183	18.622	#
C4H8O 2-BUTANONE	72.10572	-238.362			102.432	339.991		
H8C4O 2,3-Dimethyloxyrane	72.10572	-137.658	-113.00	±8.	95.471	303.780	17.777	#
OC4H8 ETHYL-OXYRANE	72.10572	-115.960	-91.115	±8	91.134	316.499	17.582	#
C4H8O Tetrahydrofuran, Oxolan	72.10572	-184.18	-156.421		76.25	302.41	14.667	
C4H8O2 1,4 DIOXANE	88.10632	-314.428		±7.	92.568	294.582		
(CH3COOH)2 Acetic Acid dimer	120.1048	-929.015	-901.62		137.254	414.396	28.053	†
C4H8O4 Tetraoxocan	120.10512	-620.2			116.255	340.343		
C4H8S Tetrahydrothiophen	88.17232	-34.1	-8.296		92.55	309.627	16.694	
1,4-C4H8S2 Dithiane	120.23952	0			109.655	326.252		*
1,3-C4H8S2 Dithiane	120.23952	-10			110.434	333.542		
C4H9,n-Butyl Radical	57.11426	81.80	105.91	±8.	94.555	307.628		#†
i-C4H9 iso-Butyl Radical	57.11426	73.785	97.92	±8.	98.111	304.662	18.063	#
s-C4H9 *sec*-Butyl Radical	57.11426	70.224	94.945	±8.	86.395	327.417	17.538	#
C4H9,t-Butyl Radical	57.11426	55.041	79.719	±8.	82.410	323.393	17.010	#
C4H9N PYROLIDINE	71.12100	-3.59	26.889	±0.8	82.112	309.206	16.177	#
C4H9NO2 Nitrobutane	103.121	-143.93	-109.63		115.119	369.874	21.040	
C4H9O n-BUTOXY RAD	73.11366	-56.350	-29.003	±8.	101.894	337.600	19.314	#
C4H9O I-BUTOXY RAD	73.11366	-65.070	-36.703	±8.	101.777	319.038	18.294	#
C4H9O S-BUTOXY RAD	73.11366	-69.84	-41.88	±8.	102.025	327.058	18.700	#
C4H9O T-BUTOXY RAD	73.11366	-86.923	-58.899	±8.	106.062	309.188	18.637	#
C4H10 n-Butane	58.123	-125.790	-98.46	±0.67	98.651	309.884	19.227	†
I-C4H10 ISOBUTANE	58.123	-134.990	-106.37	±0.63	96.643	295.493	17.936	†
C4H10FO2P SARIN	140.09437	-963.157	-927.62	±40	161.667	412.013	29.468	#
C4H10N2 1,4-Piperazine	86.13568	32.058	70.65	±8.	96.860	301.189	16.633	#
C4H10O-N 1-BUTANOL	74.1228	-274.68			108.168	361.616		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C4H10O-S 2-BUTANOL	74.1228	-292.629			111.134	363.877		
C4H10O-T 2-Methylpropanol	74.1228	-312.628			113.481	329.72		
C4H12Sn Sn(CH3)4	178.84808	-20.502	+11.004	±4.2	145.919	410.093	29.840	#
C4H12Sn H2Sn(C2H5)2	178.84808	56.484	90.910	±4.2	143.567	410.046	26.920	#
C4N2 Carbon Subnitrid	76.0574	529.2	524.285	±0.8	86.326	290.524	17.799	†
C5	60.05350	1050.924	1040.0	±60.	75.507	271.676	16.192	†
C5F12 FC 4-1-12	288.03584	-2543.311			229.036	555.108		
C5H	61.0629	778.276			65.158	260.415	12.013	*
C5H2	62.0709	691.412			82.981	266.639	14.674	*
C5H2CL2O CY	148.97418	-12.17	-5.59		111.295	349.650		#
C5H2CL3 CY	168.42748	152.68	158.05		118,207	369.726		#
C5H3 1,3-Pentadiyne-5-yl Rad.	63.07882	602.58			87.499	295.196		
C5H3 HCCCH*CCH	63.07882	564.61		±43	93.241	306.147		
C5H3 Cyclopentatriene-yl	63.07882	697.77		±75	70.898	281.721		
C5H3CL3O CY	185.43482	-104.72	-93.65	±8.	139.671	397.902		#
C5H3N HCC-CH=CH-CN	77.08406	422.613	426.538	±8.	93.766	318.598	18.380	#
C5H4 1,3-Pentadiyne	64.08526	411.835	416.818	±8.	86.669	291.342	17.221	#
C5H4 1,4-Pentadiyne	64.08526	451.964	434.773	±8.	89.940	305.243	17.191	#
C5H4 Pentane-Tetraene	64.08526	444.466	449.702	±8.	86.132	287.480	16.968	#
H4C5 1,2-Pentadiene-4-yne	64.08526	433.354	438.929	±8.	86.751	301.509	16.628	#
C5H4 1,2,4-Cyclo-Pentatriene.	64.08526	551.485		±9.	73.235	279.6		
C5H4N *CH=CH-CH=CH-CN	78.09200	502.942	510.320	±8.	97.601	341.652	19.160	#
C5H4N meta-Pyridyl Radical	78.09200	405.241	418.146	±8.	74.123	292.227	13.634	#
C5H4O Cyclopentadiene-1-one	80.08616	55.229			80.941	289.977		
C5H4O2 3 ketene	96.08556	-105.834	-95.030	±8	101.982	361.789	20.080	#
C5H5 1-Pentyne-3-ene-5-yl	65.09320	384.93	393.17	±8.	94.137	324.558	18.196	#
C5H5 CY Cyclopentadienyl Rad.	65.09320	266.102			76.605	279.485		
C5H5N CH2=CH-CH=CH-CN	79.09994	238.944	250.471	±8.	99.632	336.825	19.246	#
C5H5N PYRIDINE	79.10144	140.37		±0.54	77.746	282.759		
C5H4OH CYCLO RAD	81.0941	66.526			95.625	310.007		
1,3C5H5O CY RADICAL	81.0941	59.8			90.023	307.695		
1,4C5H5O CY RADICAL	81.0941	103.3			90.479	307.805		
2,4-c-C5H5O CY RADICAL	81.0941	221.758			83.1	302.922		*
C5H5O2 2-pentenedialdehyde R	97.0935	-83.638			110.293	391.33		
C5H5O2 2-pentenedialdehyde R	97.0935	-72.76			113.89	387.94		
C5H6 1,2,4-Pentatriene	66.10264	252.295	264.571		93.878	318.687		
C5H6 1-ene-2-yne	66.10264	249.366			89.238	320.076		
C5H6 3-enE-1-yne	66.10264	256.479			94.424	314.637		
C5H6 CYCLOPENTADIENE	66.10264	134.3	151.43	±1.5	75.368	274.152	13.535	†
C5H6N2 2-AMINOPYRIDINE	94.11612	118.616		±0.84	103.84	309.401		
2,4-C5H5OH	82.10204	7.9			91.437	304.61		
1,3-C5H5OH	82.10204	-24.3			94.957	304.343		
1,4 C5H5OH	82.10204	-27.2			95.023	304.565		
C5H7 1,3-Pentadien-5-yl	67.10908	205.455	222.877	±8.	92.672	325.606	17.484	#
C5H7 1,4-Pentadien-3-yl	67.10908	205.455	223.086	±8.	93.92	323.195	17.275	#
C5H7 Cy 1-penten-1-yl	67.10908	172.623	192.745	±8.	79.939	296.325	14.785	#
C5H7 Cy 1-penten-4-yl	67.10908	223.94	243.815	±8.	80.499	290.579	15.031	#
C5H7CL	102.56178	58.091	76.235	±8	110.072	374.067	21.352	#
C5H7CL2	138.01448	110.926	128.756	±8	132.403	444.862	26.257	#
C5H7NO	97.11672	-108.7			120.7	387.6		
C5H7O 1-Cypenten-4-oxy Rad.	83.10848	95.04	117.53	±8.	92.705	317.69		#
C5H8 1,3-Pentadiene	68.11702	84.157	105.770	±8.	94.718	318.284	17.527	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C5H8 ISOPRENE	68.11852	75.73			104.6	315.641		
C5H8 Cyclopentene	68.11852	33.9	58.183		81.275	291.379	14.857	†
C5H8CL CH2ClCH=CHCH2CH2	103.56972	158.197	179.288	±8.	119.551	399.520	22.640	#
PETN Solid	316.13828	-538.481		±0.84	353.757	101.964		
C5H8N4O12 PETN	316.13828	-387.02	-332.00		294.758	614.706	53.542	
C5H8O Cyclopentanone	84.116420	-197.401	-171.29	±5.4	97.436	309.296	17.366	#
C5H8O 1,5-Cyclopenten-2-ol	84.116420	-126.579	-99.582	±8.	96.604	315.064	16.583	#
C5H9 CY	69.12496	111.131	138.404	±8.	88.092	298.784	16.101	#
C5H9 2-PENTEN-5-YL	69.12496	174.615	196.937	±8.	110.968	357.785	21.052	#
H9C5 2-PENTEN-1-YL	69.12496	116.700	140.617	±8.	106.281	347.013	19.457	#
C5H9 3M-1-BUTEN3YL	69.12496	102.479	126.020	±8.	107.506	333.972	19.833	#
C5H9 3M-1-BUTEN1YL	69.12496	219.091	243.190	±8.	105.817	335.407	19.275	#
C5H9 3M-1-BUTEN4YL	69.12496	180.356	204.114	±8.	108.450	348.534	19.616	#
C5H9N	83.1332	75.312		±8.4	99.27	274.978		
C5H10 1-PENTENE	70.13290	-21.28	+ 4.648		108.200	347.110	21.680	†
C5H10 2-PENTENE	70.1344	-31.757			108.449	340.41		
C5H10 2MB-1ene	70.1344	-36.317			109.956	339.532		
C5H10 2MB-2ene	70.1344	-42.551			105.018	338.569		
C5H10 2MB-3ene	70.1344	-28.953			118.616	333.465		
C5H10 Cyclopentane	70.1344	-77.1	-44.515		82.760	293.007	15.023	†
C5H10O TetraHydroPYRAN	86.1338	-224.283	-189.04	±0.84	96.359	301.959	16.710	#
N-C5H11 n-pentyl	71.14234	45.81	73.23		119.150	368.649	24.422	†
S-C5H11 1-methyl-butyl	71.14234	45.564			119.653	369.949		
T-C5H11	71.14084	32.6	64.8	±8.	98.855	366.474	19.644	†
C5H11 neopentyl	71.14234	34.392			118.84	333.423		†
C5H11NO2 Nitropentane	117.14788	-164.431	-123.37	±2.1	137.100	390.905	23.792	
C5H12 PENTANE	72.14878	-146.76	-114.87		120.040	349.560	24.184	†
I-C5H12 Isopentane	72.14878	-153.70	-119.63		118.870	343.740	22.008	†
CH3C(CH3)2CH3 Neopentane	72.14878	-167.92	-135.02		120.830	306.000	23.179	†
C5H12O liquid MTBE	88.14968	-313.6	-293.85		187.510	265.650		
C5H12O Me-Tertiary Butyl Ether	88.14968	-283.7	-247.14	±0.8	138.010	355.489		#
C6 linear	72.0642	1313.	1302.33	±18.	84.585	300.600	17.770	#
C6CL6 Hexachlorobenzene	284.7822	-33.89			175.31	441.203		
C6D5 Deuterated phenyl radical	82.13651	315.700	327.525		94.997	300.504	15.919	†
C6D6 Deuterated Benzene	84.14881	58.157	73.86		100.398	282.629	16.325	†
C6F6 Hexafluorobenzene	186.05642	-956.63			157.938	384.457		
C6F14 FC 51-14Perfluorohexane	338.04364	-2949.201			269.551	629.592		
C6H	73.07394	1037.632			96.024	312.451		
C6H2	74.08188	700.82			104.103	299.19		†
C6H2CL3O Trichlorophenoxy ra	196.43758	-27.48	-20.29		140.508	398.583		#
C6H2CL3O Trichlorophenol Rad	196.43758	101.51	107.37		144.581	410.077		#
C6H2CL3O3 Peroxybiciclo Rad.	228.43638	131.42	142.99		174.462	429.942		#
C6H2CL3O3 Peroxybicyclo Rad	228.43638	28.95	40.414		171.330	433.035		#
C6H3	75.08802	682.016			100.896	319.344		
C6H3 Cy o-Benzyne-o-yl Rad.	75.08802	728.911	733.879	±8.	75.851	293.013	14.055	#
C6H3Cl3 1,3,5-trichlorobenzen	181.44612	-4.314	5.25	±8.	128.171	364.132	23.231	#
C6H3CL3O Trichlorophenol	197.44552	-189.07	-176.92		142.427	397.903		#
C6H3CL3O linear	197.44552	-19.83	+17.3		39.200	109.923		
C6H3CL3O2 CY	213.44492	-277.25	-263.99		162.216	420.242		#
C6H3I o-Iodo-Benzyne	201.99249	534.715	542.244	±12.	96.910	340.309	18.093	#
C6H3(NO2)3 Trinitrobenzene	213.10464	62.342	82.617		205.633	485.335	37.794	
1,2-C6H4 o-BENZYNE	76.09596	461.135	470.128	±8.	78.406	283.240	14.265	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
1,3-C6H4 m-BENZYNE	76.09596	523.690	532.497	±8.	80.202	283.810	14.451	#
1,4-C6H4 p-BENZYNE	76.09596	574.254	582.364	±8.	85.476	282.239	15.147	#
C6H4 TRANS	76.09596	523.105	527.104	±8.	102.894	317.187	19.328	#
C6H4 CIS	76.09596	524.218	528.632	±8.	101.969	317.563	18.843	#
C6H4 HEXAPENTAENE	76.09596	568.263	572.160	±8.	99.977	309.859	19.359	#
C6H4 TRIENE-5YNE	76.09596	559.706	563.792	±8.	101.909	325.109	19.172	#
C6H4CL –ortho Radical	111.55046	303.173		±28.9	100.842	329.678		#
C6H4CL –metha Radical	111.55046	297.02		±28.0	101.165	329.135		#
C6H4CL –para Radical	111.55046	298.86		±28.0	101.264	329.476		#
C6H4CLO o-Chlorophenoxy Rad	127.54806	30.60	43.48		109.181	344.708		#
C6H4CLO Cy " Radical	127.54806	225.91	237.50		112.226	359.349		#
C6H4CL2 o-Dichlorobenzen	147.00136	28.464	40.970	±8.	111.879	347.871	19.933	#
C6H4CL2 m-Dichlorobenzen	147.00136	22.656	35.089	±8.	112.361	343.476	20.005	
C6H4CL2 p-Dichlorobenzen	147.00136	23.104	35.493	±8.	112.303	337.735	20.049	#
C6H4CL2O Z 2,4- Dichlorophenol	163.00076	-158.009	-143.023	±8.	128.644	364.031	21.793	#
C6H4CL2O E 2,4- Dichlorophenol	163.00076	-145.398	-131.202	±8.	130.914	368.913	22.582	#
C6H4N4O2 4-Nitro-Phenyl-Azide	164.12172	389.7	410.723	±5.2	157.694	420.170	28.254	#
o-C6H4I Radical	203.00043	427.186	439.032		97.752	346.415	18.010	#
o-C6H4I2	329.90490	248.95	263.625	±5.9	113.052	386.892	21.778	#
m-C6H4I2	329.90490	243.509	257.766		118.125	384.828	22.196	#
p-C6H4I2	329.90490	242.700	257.177		114.640	365.746	21.976	#
C6H4O2 O=C6H4=O	108.09656	-122.9			108.485	333.212		
C6H5 CHAIN	77.1057	531.368			109.472	339.195		
C6H5 PHENYL RAD	77.10390	339.740	353.657	±2.5	76.656	286.072		#
C6H5 FULVENYL RAD	77.10390	467.315	479.324	±8.	87.147	297.813	15.482	#
C6H5 FULVENYL Rad. Melius	77.1057	490.365		±52.	93.077	307.123		
C6H5Br Bromobenzen	157.0079	101.253	123.571	±8.	97.507	324.774	17.433	#
C6H5BrO 2-Bromophenol (Z) cis	173.00730	-63.72	-39.09	±8.	113.188	350.929	19.051	#
C6H5BrO 2-Bromophenol-Etrans	173.00730	-70.208	-46.085	±8.	115.810	356.656	19.968	#
C6H5CL Chlorobenzen	112.55660	52.287	67.461	±8.	96.152	313.366	16.908	#
C6H5CLO o-Chlorophenol (Z)	128.55600	-130.942	-113.250	±8.	112.581	341.454	18.729	#
C6H5CLO o-Chlorophenol (E)	128.55600	-117.834	-100.912	±8.	114.787	346.205	19.500	#
C6H5CLO 2,4-Cy-hexadiene...	128.55600	-35.75	-19.81		113.199	352.445		#
C6H5CLO 2,5 Cy-hexadiene…	128.55600	-55.87	-39.79		113.969	346.868		#
C6H5F Fluorobenzen	96.10230	-113.914	-97.973	±8.	92.385	301.688	15.963	#
C6H5I Iodobenzen	204.00837	165.	181.038	±6.	99.918	334.751	18.051	#
C6H5NO NITROSOBENZENE	107.11004	198.075	215.586	±8.	106.354	332.852	18.655	#
C6H5NO2 NITRO-BENZENE	123.11124	68.534	88.137		120.38	348.800	20.903	
C6H5O PHENOXY RAD	93.10330	54.		±10.	97.682	311.871		
C6H5O Cy-hexadiene-1one-2yl	93.10330	246.58	260.42		98.386	332.759		#
C6H5OO PEROXYPHENYL rad	109.10270	141.612	158.975	±8.	108.706	339.197	18.808	#
C6H6(L)	78.11184	49.08	50.695		135.95	173.44	30.110	†
C6H6 BENZENE	78.11184	82.88	100.41		81.934	269.158	14.195	†
C6H6 FULVENE	78.11364	236.814		±10	90.362	294.123		
C6H6 BENZVALENE	78.11364	384.9	403 ?	±8.3	80.825	284.701		#
C6H6 1,5-Hexadiyine	78.11364	417.166	428.062	±8.	111.036	336.936	20.829	#
C6H6 2,4-Hexadiyne	78.11364	369.100	379.830	±8.	103.026	335.627	20.995	#
C6H6 1,3-Hexadiyne	78.11364	392.363	404.299	±8.	107.021	328.174	19.790	#
C6H6 1,2,4,5 Hexatetraene	78.11364	396.229	407.942	±8.	102.421	343.852	20.012	#
C6H6 1,2-Hexadiene-5-yne	78.11364	412.542			107.68	336.912		
C6H5OH PHENOL	94.11124	-83.847	-58.807	±8.	103.338	315.238	17.497	†
C6H6O 2,4-Cyclohexadiene1one	94.11124	-21.63	-3.31		99.188	322.935		#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C6H5OOH Hydroperoxyphenyl	110.11064	-2.678	18.039	±8.	114.440	350.539	19.688	#
C6H7 1,4 CYCLO Radical	79.11798	200.589		±35	97.618	305.835		
C6H7 1,3,5-Hexatriene-6-yl	79.11798	431.387	446.410	±8.	110.758	363.629	20.937	#
C6H7-1 CY C5H5-1-CH2*	79.11798	334.092	351.954	±6.3	100.095	326.062	18.098	#
C6H7-3 CY C5H5-3-CH2*	79.11798	247.316	265.583	±19.2	101.756	321.686	17.693	#
C6H7-1 CY C5H4-1-*-CH3	79.11798	226.773	244.638	±12.5	103.103	314.389	18.094	#
C6H5NH2(L) aniline	93.12832	31.50	37.774		191.92	191.060	34.020	†
C6H7N ANILINE	93.12832	87.04	--		108.385	319.27	--	
C6H8 DIHYDROBENZVALENE	80.12772	230.12	255.3	±8.3	89.425	293.780		#
C6H8 CY 2,4-C5H5-1-CH3	80.12772	112.257	135.267	±8.	95.574	310.854	17.183	#
C6H8 CY 2,4-C5H5-3-CH3	80.12772	102			116.8	310.3		
C6H8 1,3,5-HEXATRIENE	80.12772	152.214			107.911	330.388		
H8C6 (1,3-CYCLO)	80.12772	106.3			94.168	303.419		
C6H8 (1,4-CYCLO)	80.12772	109			94.053	296.34		
C6H9 1,3 hexadiene 5-yl Rad.	81.13566	173.49	195.692	± 8.	119.775	370.613	22.225	#
1,3-C6H9 hexadiene 6-yl Rad.	81.13566	265.533	286.651	± 8.	120.582	389.084	22.990	#
C6H9 Cyclohexenyl-3	81.13566	131.47	159.011	± 8.	97.860	313.685	16.886	#
C6H9 CY 1- C5H6-4-CH3-4-yl	81.13566	188.468	214.322	± 8.	103.489	321.009	18.574	#
C6H9 CY 1- C5H7-4-CH2*	81.13566	215.731	241.534	± 8.	106.551	323.588	18.625	#
C6H9 CY 1-C5H7-3-CH2*	81.13566	212.464	237.965	± 8.	104.037	333.573	18.926	#
C6H9 CY 1-C5H7-1-CH2*	81.13566	124.9			94.663	323.377		
C6H9I CY 1-C6H9-3-I	208.04013	69.036	99.331	±21.	116.001	360.644	20.731	#
C6H10 1,3-HEXADIENE	82.14360	58.513	84.568	±8.	120.575	372.675	22.606	#
C6H10 Cyclohexene	82.14360	-4.6	+26.79		101.464	310.632	17.271	†
C6H10 C5H7-CH3 Cypentene-4	82.14360	8.46	38.49	±8.	101.249	309.518	17.208	#
C6H11 CH2=CHC3H6CH2*	86.15334	162.502	190.886	±8.	127.963	417.768	24.512	#
C6H11 CH3CH=CHC2H4CH2*	86.15334	153.862	181.880	±8.	129.760	404.206	24.878	#
C6H11 trans 3-hexene-6-yl Rad	83.15334	154.540	183.164	±8	128.546	401.219	24.272	#
C6H11 CH2=C(CH2*)C3H7	83.15334	95.340	125.298	±8	125.511	391.885	22.942	#
C6H11 CH2=C(CH3)C3H6*	83.15334	149.787			130.797	390.786		
C6H11 CH3C(CH2*)=CHC2H5	83.15154	90.847	121.134	±8.	122.131	383.848	22.609	#
C6H11 CH3C(CH3)=CHC2H4*	83.15334	141.838			124.52	387.438		
C6H11 (CH3)2C=CHCH*CH3	83.15154	72.91	101.569	±8.	128.105	375.530	24.237	#
C6H11 (CH3)CHCH*CH=CH2	83.15154	91.232	119.916	±8.	135.913	384.042	24.212	#
C6H11 2-Methyl-1-pentene-4-yl	83.15154	136.913	165.834	±8.	127.708	386.671	23.975	#
C6H11 Cyclohexy Radical	83.15154	75.839	110.421	±8.	106.108	317.527	18.513	#
C6H11I Iodo-CycloHexane	210.05601	-50.0	-11.926	±4.7	121.960	363.668	21.420	#
C6H12 TRANS-3-HEXENE	84.16128	-50.417	-17.218	±8.	128.815	365.867	23.931	#
C6H12 1-HEXENE	84.16128	-41.95	-11.06		130.800	386.850	26.240	†
C6H12 2MP-1ene	84.16128	-59.371			135.603	382.167		
C6H12 2MP-2ene	84.16128	-66.86			126.608	378.443		
C6H12 4MP-2ene CIS	84.16128	-57.446			133.553	373.338		
C6H12 4MP-2ene TRANS	84.16128	-61.463			141.419	368.276		
C6H12 CYCLOHEXANE	84.15948	-123.3	-83.715		105.343	297.389	17.545	†
N-C6H13 n - HEXYL RAD.	85.16742	25.10	57.480		141.790	408.339	28.983	†
2-C6H13 2-HEXYL RAD.	85.16922	28.158	61.309	±8.	147.533	428.452	28.213	#
C6H13 2MP-1YL	85.16922	35.635	70.799	±8	140.892	399.411	26.200	#
C6H13 2MP-5YL	85.16922	32.367	67.427	±8.	139.391	414.154	26.304	#
C6H13-S 2ME - 4PENTYL	85.16922	20.079	55.023	±8.	141.737	402.960	26.420	#
C6H13-T 2ME 2PENTYL	85.16922	17.209	52.180	±8.	139.289	404.566	26.392	#
C6H14(L) n-Hexan	86.17716	-198.660	-179.98		195.480	296.090	46.920	†
C6H14 n-Hexane	86.17716	-166.92	-130.02		142.59	388.85	28.702	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
H14C6 2-METHYLPENTANE	86.17716	-174.55			142.21	380.98		
C6H14 3MP	86.17716	-171.97			140.21	383.03		
C6H14 2,2-DMBUTANE	86.17716	-184.68			141.46	358.34		
C6H14 2,3-DMBUTANE	86.17716	-176.8			139.41	365.92		
C6H14O (L) 1-Hexanol (liq)	102.17476	-377.5		±0.44	243.2	287.4		X
C6H14O 1-Hexanol	102.17476	-314.7	-269.230	±1.4	139.043	376.040	24.468	#
C6N6O6 BENZOTRIFUROXAN	252.10284	N/A	N/A		200.972	416.395		
C7 linear	84.0749	1326.33	1313.33	±18.	98.927	314.106	20.372	#
C7F16 Perfluoroheptane	388.05145	-3383.969			300.804	704.075		
C7H4	88.10666	676.13	682.585		100.798	312.080		#
C7H5N C6H5-CN Benzonitrile	103.12134	213.066	227.443	±8.	105.310	328.810	18.503	#
TNT Solid	227.13122	-63.178		±5.0	244.68	137.779		
C7H5N3O6 TNT	227.13122	24.1	53.992	±8.4	215.417	481.936	37.698	#
C7H5N5O8 Tetryl Solid	287.1456	41.003			290.913	143.469		
C7H6O BENZALDEHYDE	106.12404	-36.8			111.673	336.019		
C7H7 2,4,6-Cycloheptatriene-1-yl	91.13048	280.696	298.308	±8.	109.167	332.619	19.401	#
C7H7 BENZYL RADICAL	91.13048	208.0	226.8	±1.9	109.700	318.229	18.178	#
C7H7 Quadricyclene Appex Rad.	91.13048	534.519	556.275	±2.2	95.877	297.781		#
C7H7 Quadricyclene Basis Rad.	91.13048	581.346	603.316	±2.2	90.683	299.778		#
C7H7 Quadricyclene Shoulder R	91.13048	588.94	611.424	±2.2	90.774	299.687		#
C7H7O C_6H_5-CH_2O*	107.12988	125.909	146.9	±8.	117.167	351.816	20.362	#
TOLUENE(L)	92.13842	12.18	19.957		157.29	221.030	33.470	†
C7H8 TOLUENE	92.13842	50.17	73.476		103.279	320.187	17.940	†
C7H8 Norbornadiene	92.14052	247.6			96.748	295.226		
C7H8 (liq) Quadricyclene	92.13842	302.1		±2.2	----	----		X
C7H8 Quadricyclene	92.13842	337.23	363.987	±2.2	91.551	228.420		#
C7H8 1,3,5-Cycloheptatriene	92.14052	182.8			106.251	316.365		
C7H8 1,6-Heptadiyne	92.14052	395.8			134.202	379.7		
C7H8O CRESOL	108.13782	-132.298	-108.55		128.026	360.116	21.838	†
C7H8O BENZYL-ALCOHOL	108.13782	-94.6	-70.081	±3.0	119.290	360.634	21.068	#
C7H10 3,5-dimethyl-CPD	94.1564	66.7			142.3	341.9		
C7H10 NORBORNENE	94.15640	90.	73.69	±30.	103.136	306.087		
C7H10N2O2 Cyclo(Pro-Gly)	154.16658	-341.012	-301.25	±12.5	158.210	401.299	27.301	#
C7H12 NORBORNANE	96.17228	-53.723		±8.4	103.291	307.66		#
C7H12 CY-HEPTENE	96.17018	-7.866	30.578	±8.	120.515	324.394	19.739	#
C7H13 Cycloheptanyl Radical	97.17812	77.739	118.315	±8.	126.683	353.102	21.841	#
C7H13 1-Heptyl-4/5 ene	97.17812	132.2	194.632		148.532	435.136	--	
C7H13 1-Heptene-4-yl	97.17812	129.7	192.117		149.900	505.000	--	
C7H14 n-HEPTENE	98.18816	-62.76	-26.9		153.500	425.600	30.790	†
C7H14 CY-HEPTANE	98.18816	-118.2			131.171	336.512		
C7H15 n-HEPTYL RAD.	99.1940	4.39	41.732		164.430	448.029	33.543	†
C7H15 NEOHEPTYL-1	99.1961	3.347	44.329		164.117	426.788	29.704	#
C7H15 NEOHEPTYL-2	99.19400	-2.926	37.433	±8.	168.595	430.562	30.526	#
C7H15O 3,3dimethyl1-pentanoxy	115.1955	-142.256			171.86	328.026		
C7H16(L) n-Heptan	100.20194	-224.35	-201.87		224.980	328.560	52.640	†
C7H16 n-HEPTAN	100.20194	-187.78	-145.88		165.180	429.099	33.221	†
C7H16 iso-Heptan	100.20194	-194.600	-150.40		164.500	420.500	30.920	†
C7H16 NEOHEPTAN	100.20194	-209.87			166.955	395.221		
C7H15OH n-Heptanol	116.20344	-339.741		±1.6	178.605	480.449		
C7H15OH Neoheptanol	116.20344	-359.657			179.907	448.901		
C8H CH≡C-C≡C-C≡C-C≡C*	97.09594	1162.06			132.416	358.74		
C8H2 CH≡C-C≡C-C≡C-C≡CH	98.10388	934.287			132.638	347.69		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C8H5 CH≡C-CH=CH-CH=C*-C≡CH	101.12530	808.453	812.494	±8.	141.494	402.387	26.558	#
C8H6 C_6H_5CCH	102.13564	328.151			115.734	327.918		
C8H6 Benzocyclobutene	102.13324	410.015	426.377	±8.	105.597	312.114	17.471	#
C8H6O BENZOFURANE	118.13264	17.0	37.048	±1.5	111.964	326.193		#
C8H6O2 Benzodioxin	134.13204	-71.2	-49.95	±6.	128.967	347.408		#
C8H6S BENZOTHIOPHENE	134.20164	166.272			131.558	337.481		
C8H7 STYRENE RADICAL	103.14358	389.112			127.45	344.397		
C8H7 1,3,5,7Cy-octateraene-1-yl	103.14118	503.921	522.020	±8.	118.407	340.591	19.948	#
C8H7 2,3,5,7Cy-octateraene-1-yl	103.14118	503.795	521.914	±8.	118.425	340.577	19.948	#
C8H7N INDOLE	117.15032	156.5		±1.25	121.264	332.373		
C8H8 CUBANE	104.14912	651.7		±30	98.47	271.426		
C8H8 STYRENE	104.14912	148.3	169.66	±2.	120.190	344.770	20.940	†
C8H8 1,3,5,7 Cyclooctateraene	104.14912	297.6	319.294	±1.3	122.616	327.102	20.607	#
C8H8 2,3,5,7 Cyclooctateraene	104.14912	389.434	411.499	±8.	118.990	338.828	20.235	#
C8H8 Benzocyclobutane	104.14912	200.476	224.662	±8.	109.342	317.617	18.115	#
C8H9 $C_6H_5CH_2CH_2$*	105.15706	237.714	262.114	±8.	130.543	364.717		#
C8H10 C6H5C2H5	106.1650	29.790	58.81	±8.	129.799	353.746		†#
C8H10 Di METHYLBENZENE	106.16699	17.994	-----		125.745	352.115	21.974	*
C8H14 CH(-CH_2-CH_2-)$_3$CH	110.19676	-99.035	-51.705	± 1.	125.174	327.572	20.374	#
C8H15 1-Octen-4-yl	111.20710	109.1	181.039		172.717	481.400	---	
1-C8H16 1-OCTENE	112.2144	-83.59	-42.768		176.100	464.840	35.350	†
C8H16 CycloOctane	112.21264	-124.4	-72.762	± 1.	146.194	366.725		#
N-C8H17 N-OCTYL RAD	113.2223	-16.32	+25.983		187.070	488.879	38.103	†
C8H18(L) n-Octane	114.22852	-250.260	-227.11		254.150	361.071	61.490	†
C8H18 OCTANE	114.22852	-208.75	-161.89		187.780	468.480	37.780	†
C8H18(L) isooctane	114.22852	-259.160	-224.71		239.000	328.110	50.190	†
C8H18 ISO-OCTANE	114.22852	-224.01	-171.54		188.410	423.090	32.170	†
$(CH_3)_3$C-OO-C$(CH_3)_3$ Liquid	146.22732	-380.8	---	±2.0				X
C8H18O2 $(CH_3)_3$C-OO-C$(CH_3)_3$	146.22732	-343.	---		219.150	482.400	---	
C8H20Pb $(C_2H_5)_4$Pb Liquid	323.4444	53.0		±5.				X
C8H20Pb $(C_2H_5)_4$Pb Gas	323.4444	109.6	169.315	±5.1	233.217	477.890		#
C9H4 $C(CCH)_4$	112.12806	913.78	918.435		126.858	330.747		#
C9H7 INDENYL	115.15188	285.6	304.521	±22	128.21	342.843	20.199	#
C9H7N QUINOLINE	129.15862	200.52	223.454		129.153	344.075	20.521	#
C9H7N ISOQUINOLINE	129.15862	204.61	227.487		128.983	344.568	20.578	#
C9H8 INDENE	116.15982	164.138	187.693	±1	124.226	335.846	19.799	#
C9H10 METHYLSTYRENE	118.1784	112.968			146.858	383.673		
C9H12 C(CH=CH_2)$_4$	120.19158	250.6	279.18		174.032	417.887	31.734	#
C9H12 1,3,5-Trimethylbenzene	120.19158	-16.067	44.22 ?		147.800	385.300	---	
C9H12 1,2,4-Trimethylbenzene	120.19158	-13.933	46.36 ?		154.508	395.765	---	
C9H12 Propylbenzene	120.19158	7.95	68.240		151.461	399.990	---	
C9H17 1-Nonenyl Radical	125.23398	88.400	169.860		195.709	520.900	---	
C9H18 1-Nonene	126.24192	-432.207			200.269	505.000		
C9H18O6 cyTriAcetoneTriPeroxy	222.23562	-395.472	-331.52	±22	302.788	499.584	47.780	#
N-C9H19 n-NONYL RAD	127.2491	-37.03	+10.234		209.710	527.419	42.664	†
N-C9H20 liq. NONANE	128.2578	-275.475			284.386	393.673		
N-C9H20 NONANE	128.2578	-228.907	-177.09		210.413	506.431	42.342	
C10D8 NAPHTHALENE-D8	136.22281	118.111			156.96	350.669	23.646	*
C10H6 Naphtyne	126.15764	500.825	515.5		132.178	347.542	21.264	
C10H7 Naphtyl Radical	127.16558	396.225	415.418		132.216	352.133	20.980	
C10H7 C_6H_5CH=CH-C≡C*	127.16558	687.515	701.677	±20	144.738	406.909	26.011	#
C10H7 C_6H_4*CH=CH-C≡CH	127.16558	630.612	645.066	±20	148.770	402.203	25.719	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C10H7 $C_6H_4(C_2H)CH=CH$*	127.16558	617.140	634.110		144.841	367.587	23.203	
C10H7I (L) 1-Iodobenzene Liq.	254.06705	162.		±6.3				X
C10H7I 1-Iodobenzene	254.06705	234.	----	±8.8	158.574	394.133	-----	
C10H7O* Naphthol Radical	143.15498	115.478	136.47		146.882	373.015	23.522	
H8C10 AZULENE	128.17352	279.932			128.868	338.065	20.368	*
C10H8 NAPHTHALENE	128.17352	150.582	174.276	±1.5	131.920	333.267	20.713	†
C10H8O Naphtol	144.17292	-30.794	-6.37		154.318	368.709	24.318	#
C10H9 2-HydroNaphthalen Rad	129.17846	229.534	255.533		143.289	363.659	22.643	
C10H9 $C_6H_5CH=CHCH=CH$*	129.17846	444.508	466.692	±20	152.314	419.069	26.458	#
C10H9 1-Methyl-1-Indenyl Rad	129.17846	262.337	287.549	±20	144.004	369.098	23.429	#
C10H9 1-Methylene-Indene Rad	129.17846	337.649	363.520	±20	144.045	364.065	22.771	#
C10H9 2-Methylene Indene Rad	129.17846	266.5		±20	-	-		X
C10H10 1,2-DihydroNapthalene	130.1864	117.152	147.213		143.955	359.383	22.797	
C10H10 1,1'-BiCyclo-Pentadiene	130.1864	291.625	320.336		143.016	385.011	24.164	#
C10H10 2,2''-BiCycloPentadiene	130.1864	291.056	318.773		150.301	386.504	25.159	#
C10H10 1-Methyl Indene	130.1864	184.933	214.695	±20	144.346	360.391	23.113	#
C10H10 2-Methyl Indene	130.1864	173.636	202.811	±20	146.240	364.509	23.701	#
C10H10 3-Methyl Indene	130.1864	173.218	202.400	±20	146.056	364.755	23.694	#
C10H13 C5H7-C5H6*	133.21322	197.15	----	±20	149.452	395.356	---	
C10H14 3,3-C5H7-C5H7 bicyclo	134.21816	108.784	152.131	±20	155.753	401.109	26.465	#
11-C10H15 JP-10 apex Radical	135.22910	105.650	157.726		142.526	359.233	21.970	#
6-C10H15 JP-10 Tert side Rad.	135.22910	96.32	149.14		138.190	355.345	21.225	#
C10H15 C5H8*-C5H7	135.22910	171.54	218.396	±125.5	155.918	417.467		
C10H16 JP-10	136.23404	-86.856	-31.374		152.560	359.201	22.997	†
C10H19 1-Decenyl 4/5 Radical	139.26086	67.900	158.882		218.653	560.300	-----	
C10H19 1-Decenyl 3 Radical	139.26086	2.600	93.582		221.077	567.300	-----	
C10H20 1-Decene	140.26880	-123.900			223.362	544.500		
C10H20 2-Decene-trans	140.26880	-136.200			222.222	541.000		
C10H20 3-Decene-trans	140.26880	-135.500			220.659	542.600		
N-C10H21 n-DECYL 1-Radical	141.27374	-57.74	-5.514		232.350	567.109	47.224	†
C10H21 n-Decyl – 2-Radical	141.27674	-58.100			230.534	567.300		
C10H21 n-Decyl-3/4 Radical	141.27674	-58.200			230.534	567.300		
N-C10H22 liq DECANE	142.28468	-301.039			314.511	425.889		
N-C10H22 gas-DECANE	142.28468	-249.534	-192.75		233.049	545.677	46.903	
1-C10H7C*O Naphtaldehyde Rd.	155.17598	174.891	193.741		161.693	399.949	26.717	
1-C10H7CHO Naphtaldehyde	156.18392	30.543	54.59		162.397	383.881	25.754	
1-C10H7-CH2* Methyl-Naphthyl	141.19246	272.797	297.846		158.090	378.770	24.645	
1-C10H7-CH3 MethylNaphthalen	142.20040	116.106	145.0		157.922	381.348	25.026	
C11H24 N-UNDECANE	156.31156	-270.286	-208.54		255.684	584.923	51.463	
O-C12D9 O-BIPHENYL Radical	162.25892	386.58			195.578	428.768		*
C12D10 BIPHENYL – D	164.27302	138.488	162.92		200.307	413.489		*
C12H4CL4O 2,3,6,7	305.97036	-50	-35.924	±10	225.108	496.028	38.205	
C12H4CL4O 2,4,6,8	305.97036	-58	-44.108	±10	225.552	493.238	38.388	
C12H4CL4O2 2,3,7,8	321.96976	-136.1	-120.71	±10	241.524	513.049	41.226	#
C12H4CL4O2 1,3,6,8	321.96976	-174.10	-158.934	±10	241.685	520.954	41.454	#
C12H4CL4O2 1,3,7,9	321.96976	-174.130	-158.961	±10	241.657	520.551	41.452	
C12H4CL4O3 1,3,6,8	337.97276	-295.37	-278.36		256.811	533.525	43.948	
C12H4CL5O2 spiro radical	357.42246	-95.550	-80.345	±10	264.387	571.035	46.006	#
C12H4CL5O2 6-2' ether radical	357.42246	-125.900	-112.30	±10	266.495	600.066	47.612	#
C12H4CL6O2 2-6' ether	392.87516	-201.95	-187.778	±10	287.872	625.238	51.630	#
C12H4CL6O2 Biphenyl-diol	392.87876	-321.92	-305.6	±33.5	286.707	573.925	49.483	
C12H5CL3O3 2,4,7 trichloro	303.52800	-348.99	-329.03		241.279	505.020	40.642	

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C12H5CL4O2 6-6' ether radical	322.98130	-85.52	-69.659	±25.1	250.467	582.730	44.993	
C12H5CL4O3 radical	338.97710	-432.42	-412.55	±62.8	265.578	551.043	45.331	
C12H5CL4O3 radical	338.97710	-321.79	-301.82	±62.8	263.787	550.127	45.226	
C12H5CL5O2 6-6' ether	358.43040	-265.590	-247.196	±10.	272.572	577.900	47.051	#
C12H6CL2O DCDF	237.08084	5.2	25.245	±24.7	192.255	439.242		#
C12H6CL2O2 DCDD	253.08024	-89.3	-67.92	±26.6	209.088	461.386		#
C12H6CL4O2 6-2' ether	323.98564	-207.57	-187.21		256.821	561.466	44.729	
1-C10H7-C≡C* EthynylNaphthyl	151.18758	694.962	710.644		162.077	397.847	26.598	
C12H8 Acenaphthylene	152.19552	259.7		±5.9	154.775	358.632		
C10H7-C≡CH EthynylNaphthalen	152.19552	379.070	398.592		169.895	391.974	26.992	
C12H8O Di-Benzo-Furan	168.19492	55.2	80.812	±4.8	163.566	375.274	25.229	
C12H8O2 Di-Benzo-p-Dioxin	184.19432	-50.1	-23.24	±2.2	180.004	396.647	28.336	#
1-C10H7-CH=CH* Vinyl-Naphthy	153.20346	469.863	492.963		172.891	404.234	27.649	
1-C10H7-C*=CH2	153.20346	412.208	434.879		175.034	407.260	28.077	
O-C12H9 O-BIPHENYL RAD	153.2031	427.73	451.889		163.048	405.110	26.589	†
C12H9CL	188.65616	148.55			178.868	433.51		
C12H9N CARBAZOLE	167.2102	200.7			176.877	388.305		
1-C10H7-CH=CH2	154.21140	215.058	242.302		173.671	400.851	27.738	
C12H10 BIPHENYL	154.21140	182.13	210.329	±0.7	166.179	388.941	26.783	†
C12H10 1-C10H7-CH2CH2*	155.21934	292.88	322.861		185.266	418.370	29.235	
C12H10 1-C10H7-CH*-CH3	155.21934	220.497	250.340		184.272	426.717	29.373	
1-C10H7-C2H5 EthylNaphthalen	156.22728	96.901	131.723		181.943	406.323	28.829	
C12H12O 1-C10H7CH2CH2OH	172.22668	-52.718	-16.807		195.002	447.806	31.880	
C12H23 liquid JET-A(L)	167.31102	-303.469	--		350.336	448.112	--	†
C12H23 JET-A	167.31102	-211.46	--		293.494	612.539	--	†
C12H26 N-DODECANE	170.33844	-290.872	-224.17		278.32	624.253	56.024	
C12H26O (liq.) 1-Dodecanol	186.33424	-528.5	--	±0.8	438.42			X
C12H26O 1-Dodecanol	186.33424	-775.714	-648.646		294.554	674.879	--	
C13H9N ACRIDINE	179.2212	273.9			177.643	394.998		
C13H9N PHENANTHRIDINE	179.2212	240.5			184.131	391.6		
C13H28 n-TriDecane (liquid)	184.36142	-377.7		±1.6				X
C13H28 n-TriDecane	184.36142	-311.5	-179.251	±1.6	303.340	661.449	--	
C14H6(NO2)6 solid HNS	450.23068	58.07		±10.				X
C14H6(NO2)6 HexaNitroStilbene	450.23068	238.4	285.396		411.150	773.618	71.248	#
C14H10 ANTHRACENE	178.2334	230.1			184.993	392.693		
C14H10 PHENANTHRENE	178.2334	207.1			186.787	394.614		
C14H12 solid t-Stilbene	180.24508	136.73		±10.				X
C14H12 trans-Stilbene	180.24508	223.3	255.957	±4.	203.066	447.878	32.901	#
C14H14 BIBENZYL	182.26096	135.6	175.94	±1.3	202.411	477.207	33.684	#
C16H10 PYRENE	202.2554	225.7	---		202.501	407.513	--	
C16H33 2-HEXADECYL Rad.	225.43802	-181.67	-25.09?		366.100	818.976	--	#
C16H34 n-HEXADECANE	226.44596	-374.51	-213.7?		370.284	780.943	--	#
C18H12 Naphthacene	228.28788	302.	337.48	±15.	227.829	440.252	34.291	#
C18H12 (s) Triphenylene solid	228.28788	146.5		±1.5				X
C18H12 Triphenylene	228.28788	278.0	312.98	±10.	227.580	446.288	34.792	#
C20H10 Corannulene	250.29340	463.712	495.843	±7.3	216.018	412.967	31.264	#
C20H12 Perylene	252.30938	306.0	340.0	±0.8	254.201	475.499	37.878	#
C20H14 Alpha BiNaphtyl	254.32516	315.055	395.402		278.654	513.795	----	
C22H14 Pentacene	278.34656	389.000	428.03	±15.	277.388	494.673	41.423	#
C22H14 Pentafene	278.35315	345.000			282.920	501.187		
C24CL12 Perchloro-coronene	713.68920	146.6	146.7	±35.	458.824	803.678	80.264	#
C24H12 Coronene	300.35208	307.5	345.262	±10.	262.602	458.935	38.331	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
C24H17 Triphenylbenzene Rad.	305.39898	623.2			323.134	652.000		
C24H18 Triphenylbenzene	306.39972	373.38	432.36	±15.	320.200	604.870	51.514	#
C60 Buckminster Fullerene	720.66	2585.7		±105.	560.816	591.403		
C70 Footballene	840.77	2652.	2660.33	±34.	558.171	589.537		#
JET-A(L)	167.31102	-303.469	-		350.336	448.112	-	†
JET-A(G) (C12H23)	167.31102	-211.46	-		293.494	612.539	-	†
Ca (S) REFERENCE ELEMENT	40.07800	0.	0.		25.75	42.536		‡
Ca (gas)	40.07800	177.8	177.386	±0.8	20.786	154.887		†
Ca+	40.07740	773.2		±0.2	20.786	160.650		
CL	35.4527	121.302	119.633	±0.008	21.838	165.192		†
DCL	37.4668	-93.359	-93.333	±0.21	29.170	192.773	8.661	*†
DOCL	53.4662	-78.539	-76.648	±2.1	38.585	240.321	10.325	*†
CLF	54.4511	-50.293		±0.42	32.082	217.939		*
CLF3	92.44791	-158.851		±2.9	63.996	281.633		*
CLO	51.4521	101.218		±2.1	31.558	226.646		*†
CLO2 (OClO)	67.4515	104.599		±6.3	42.003	257.213		*†
CLOO	67.4518	96.238			43.982	264.994		*
CLO3F	102.4493	-23.799	-15.076		64.927	278.989	13.299	†
CL2 REFERENCE ELEMENT	70.9054	0	0		33.949	223.082		*‡
CL2O	86.9048	87.868		±6.7	47.884	267.976		*†
CL2O2	102.9042	138.976			65.034	295.883		
Cr(cr) REFERENCE ELEMENT	51.9961	0	0		23.434	23.618		*‡
Cr	51.9961	397.48		±4.2	20.786	174.313		
CrCl	87.4488	129.9	129.159	±2.7	34.684	249.790	9.389	#
CrClO		-117.9		±9.6		301.01	13.574	X
CrClO2		-310.3		±21.6		309.81	14.449	X
CrCl2	122.9015	-117.6	-120.00	±1.7	59.00	319.36	15.638	X
CrCl2O		-336.5		±22.5		333.03	16.784	X
CrCl2O2	154.90030	-519.2	-515.35	±4.2	84.052	329.53	18.066	#
CrCl3		-283.		±6.1		347.03	19.101	X
CrCl3O		-507.8		±3.0		357.32	20.049	X
CrCl4		-396.5		±13.8		371.92	22.480	X
CrCl5		-389.6				407.16	26.602	X
CrCl6	264.71230	-345.3	-344.58	+50. ?	143.573	414.95	30.878	#
CrN(s)	66.00284	-117.294		±8.4	51.093	37.215		*
CrN	66.00284	505.022		±20.9	30.753	230.553		*
CrO	67.9955	188.285		±41.8	31.33	239.27		*
CrO2	83.9949	-75.313		±41.8	43.404	269.245		*
CrO3	99.9943	-292.88	-318.00	±41.8	56.124	266.201	13.040	*
Cr2N(s)	117.99894	-125.532		±12.6	66.318	64.921		*
Cr2O3(s)	151.9904	-1135.094		±8.4	120.644	79.812		*
Cr2FeO4	223.8348	-1458.124			133.69	141.963		
Cr3C2(S)	180.0103	-85.354			99.326	85.437		
Cr7C3(S)	400.0057	-160.666			209.764	200.999		
C6Cr23	1267.9763	-328.444			628.117	612.119		
D	2.0141	221.717	219.804	±0.001	20.786	123.352	6.197	†
D+	2.01355	1540.320	1532.210	±0.001	20.786	117.585	6.197	†
D-	2.01465	142.753	147.037		20.786	117.592	6.197	†
DF	21.01251	-276.228	-276.17	±0.8	29.139	179.704	8.638	*†
HD	3.02204	0.322	0.332		29.200	143.801	8.509	†
HD+	3.02149	1496.793	1490.50		29.334	155.552	8.614	†
HDO	19.02144	-245.280	-242.35		33.798	199.517	9.926	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
HDO2	35.02084	-140.242	-134.38		43.779	243.581	11.335	†
OD	18.01350	37.226	36.852		29.939	189.666	8.999	†
OD-	18.01405	-145.378	-139.2		29.143	178.409	8.642	†
DO2	34.0129	6.487	9.387		35.845	232.883	10.065	†
SD	34.080102	140.14	140.17	±0.52	29.239	198.212	8.666	#
D2 REFERENCE ELEMENT	4.0282	0	0		29.195	144.96	8.569	‡
D2+	4.02766	1498.586	1492.29		29.510	156.735	8.651	†
D2-	4.02875	235.161	241.213		30.315	158.261	8.714	†
D2O	20.0276	-249.209		±0.067	34.256	198.342	9.960	†
D2O2	36.027	-144.3	-138.61		45.252	242.085	11.563	†
D2S	36.0942	-24.047	-21.114	±0.8	35.795	215.316	10.089	†
ELECTRON GAS e-	0.00055	0	0		20.786	20.979	6.197	*‡
F	18.9984	79.39	77.274	±0.3	22.747	158.752	6.518	†
FO	34.9978	111.267	110.632	±0.69	31.995	216.396	9.388	†
FO2 O-F-O	50.9972	378.6	381.154	±20	41.126	251.289	10.538	†
FO2 F-O-O	50.9972	25.4		±2	44.453	259.511	11.256	†
F2 REFERENCE ELEMENT	37.99681	0	0		31.304	202.792	8.825	†
F2O F-O-F	53.99621	24.5	26.754	±2	43.495	247.508	10.912	†
F2O2 F-O-O-F	69.99561	32.87	36.597	±1.3	62.073	277.214	13.778	†
Fe(a) REFERENCE ELEMENT	55.847	0	0		25.094	27.321		*‡
Fe	55.847	415.5		±1.3	25.675	180.49		
Fe+	55.84645	1181.144			26.068	181.859		
Fe-	55.84755	393.338			25.023	180.2		
FeCL	91.2997	251.036		±84.	38.245	257.577		*
FeCL2(s)	126.7524	-341.841		±0.42	76.707	117.954		*
FeCL2	126.7524	-141		±2.1	57.624	299.297		*
FeCL3(s)	162.2051	-399.405		±0.84	96.651	142.338		
FeCL3	162.2051	-253.12		±5	77.78	344.226		*
FeO(s)	71.8464	-272.037			49.972	60.754		*
FeO	71.8464	251.047		±20.9	31.415	241.926		*
Fe(OH)2(s)	89.86168	-574.059		±2.9	97.079	87.875		*
Fe(OH)2	89.86168	-330.536		±2.1	71.505	283.092		
Fe(OH)3(s)	106.86902	-832.627		±12.6	101.928	104.627		*
FeS(a)	87.913	-101.818		±0.8	50.214	59.883		*
FeS(G)	87.911	370.767			34.002	252.344		
FeSO4(s)	151.9106	-928.877		±8.4	100.666	120.949		*
FeS2(s)	119.979	-171.549		±2.1	62.18	52.926		*
Fe2CL4	253.5048	-431.374		±4.2	125.966	464.528		*
Fe2CL6	324.4102	-654.378		±8.4	173.665	536.945		
Fe2O3(S) Solid-A Hematite	159.6882	-824.248			103.866	87.404		
Fe3C (S) Solid-A	179.546	25.104			105.868	104.6		
Fe3O4(S) Solid-A Magnetite	231.5326	-1118.383			150.73	146.147		
GeBr	152.5140	137.438	144.470	>±4.2	37.250	257.225	9.864	†
GeBr2	232.4180	-60.963	-46.00	±5.	55.757	319.172	14.193	†
GeBr3	312.3220	-119.031	-96.164	>±50.	78.139	363.175	18.549	†
GeBr4	392.2260	-291.	-261.29	±6.	101.687	396.195	23.963	†
GeCl	108.0627	69.030	68.66	±18.	36.990	245.904	9.599	†
GeCl2 singlet	143.5154	-166.9	-166.39	±5.	53.806	296.332	13.307	†#
GeCl2 triplet	143.5154	102.3	102.525	±5.	54.217	307.835	13.593	#
GeCl3	178.9681	-234.4	-233.69	±5.	76.149	338.232	17.700	†#
GeCl4	214.4208	-500.9	-498.55	±5.	95.975	348.572	21.150	†#
GeH3Cl	111.08652	57.70	67.63	±5.	54.795	273.113	11.995	#

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
GeH4	76.64176	90.3	101.125	±5.	45.011	217.303	10.748	†#
H	1.00794	217.998	216.034	±0.001	20.786	114.718	6.197	†
H+	1.00739	1536.244	1528.084	±0.001	20.786	108.948	6.197	†
H-	1.00849	139.031	143.246	±0.001	20.786	108.961	6.197	†
HBr	80.91194	-36.29	-28.45	±0.16	29.141	198.699		
HCL	36.46094	-92.31	-92.125	±0.10	29.136	186.901		
HOCL	52.46004	-75.741	-72.8		37.285	236.587		
HF	20.00634	-273.3	-273.25	±0.7	29.137	173.778		
HOF	36.00574	-96.898	-94.		35.94	226.757		
HI	127.91241	26.5	28.676	±0.1	29.153	206.589		*
HNO	31.01408	106.842	109.809	±0.125	33.880	220.920	9.942	†
HNO2	47.01348	-78.452	-72.8	±0.6	46.320	254.071	11.597	†
HNO3	63.01288	-134.3	-124.58	±0.5	54.092	266.816	11.876	#
OH	17.00734	37.3	37.1	±0.3	29.886	183.737	8.813	#
OH A $^2\Sigma^+$ (excited)	17.007340	430.5	425.189		29.153	179.131	13.887	#
OH+	17.00679	1299.213	1292.987	±0.042	29.196	182.746	8.603	†
OH-	17.00789	-145.256	-139.091	±0.036	29.141	172.542	8.606	†
HO2	33.00674	12.552			34.893	229.106		†
HPO	47.9811	-56.869			35.81	235.685		
SH	33.07394	141.87	141.212	±0.52	32.446	195.751	9.274	#
SOH	49.07334	-20.895		±42	36.707	239.818		
HSO	49.07334	-4.782		±7.3	37.659	242.486		
HO2S	65.07274	-255.88		±6	50.708	276.742		
HSO3	81.07214	-385			67.209	294.061		
HS2 Hydrothiosulpheno Radical	65.13994	104.60	107.145	±10.46	39.703	253.304	10.484	#
H2 REFERENCE ELEMENT	2.01588	0	0		28.836	130.679		*‡
H2F2	40.01269	-569.924	-566.5		58.132	260.905		
H2O(L)	18.01528	-285.83			75.351	69.939		†
H2O	18.01528	-241.826		±0.04	33.588	188.829		†
H2O2(L)	34.01468	-187.778	-193.58		89.328	109.604	22.949	†
H2O2	34.01468	-135.88	-129.89	±0.2	42.416	234.542	11.162	#
H2S	34.08188	-20.6			34.248	205.803		
H2SO4(L)	98.07948	-814.01			138.594	156.907		*†
H2SO4	98.07948	-732.7	-720.85	±2.0	90.235	311.333.	18.391	#
H2S2	66.14788	15.500	21.243		48.745	251.070	11.549	
H3F3	60.01903	-883.677	-873.		73.884	280.947		
H3O+	19.02267	603.417	604.215	±1.05	35.485	193.139	10.046	†
H4F4	80.02537	-1186.932	-1174.		104.022	350.016		
H5F5	100.03172	-1490.188	-1475.		134.161	417.286		
H6F6	120.03806	-1805.545	-1788.		163.735	486.619		
H7F7	140.0444	-2099.699	-2080.		194.438	548.654		
He REFERENCE ELEMENT	4.0026	0	0		20.786	126.154	6.197	*‡
He+	4.00205	2378.519	2372.322	±0.001	20.786	131.915	6.197	†
Hg(L) REFERENCE ELEMENT	200.5900	0	0		27.978	76.028		
Hg (gas)	200.5900	-61.38	-64.53	0.04	20.786	174.972		†
HgBr2 (solid)	360.398	-169.457			75.312	170.778		†
HgBr2 (gas)	360.398	-85.452			60.319	320.239		†
HgCl (gas) Calomel	236.0427	78.45			36.34	260.0		
HgCl2 (solid)	236.0427	-230.12						
HgCl2 (liquid)	236.0427	-213.22						
HgCl2 (gas) from 1500 K and up	271.4954	-146.29			----	-----		
HgO (solid)	216.5894	-90.789	-86.208	0.1	44.132	70.282		†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
I	126.90447	106.76	107.161	±0.04	20.786	180.789	6.197	
INO2 NITRO-IODINE	172.91001	60.25		±4.2	59.366	294.432		
IO	142.90387	126		±18	33.117	239.835		
IO2 O-O-I	158.90327	116.5		±40	48.727	296.374		
IO2 O-I-O	158.90327	159.3		±25	46.697	281.231		
IO3	174.90267	241.9		±50	61.56	292.975		
I2	253.8089	62.444	65.500	±0.08	36.889	260.584	10.116	*
I2O I-I-O	269.80834	106.7		±40	52.359	330.647		
I2O I-O-I	269.80834	119.5		±25	51.874	308.111		
K(S) REFERENCE ELEMENT	39.09830	0	0		29.6	64.680		‡
K (gas)	39.09830	89.0	89.82	±0.4	20.786	160.470		†
K+	39.09775	514.0		±0.4	20.786	154.578		
KNO3(S)	101.10320	494.0	-488.31	±0.5	95.060	132.900		†
KNO3	101.10320	-315.833	-307.31		68.358	311.473	15.917	†
K2O	94.19600	-74.09	-87.945		54.180	286.548		†
K2O2	110.19540	-191.566	-207.86		70.589	306.461		†
Kr REF ELEMENT	83.8	0	0		20.786	164.086	6.197	*‡
Kr+	83.79945	1356.954	1350.76	±0.001	20.786	175.613	6.197	†
Mg (S) REFERENCE ELEMENT	24.30500	0	0		24.775	32.535-		‡†
Mg(L)	24.30500	4.79		?	---	---		
Mg (G)	24.30500	-147.10	145.90	±0.8	20.786	148.649		†
Mg+	24.30445	891.047	883.65	±1.3	20.786	154.412	6.197	†
MgAl2O4 (S)	142.26568	-2299.11			116.163	88.781		†
MgAl2O4 (L)	142.26568	-2106.53			---	---		†
MgBr	104.2090	-35.34	-27.7	±41.8	35.645	244.952		†
MgBr2(S)	184.1130	-524.6		±2.1	73.298	117.143		†
MgBr2(L)	184.1130	-490.41			----	---		†
MgBr2	184.1130	-302.92		±10.5	58.720	301.048		†
MgCO3(S) Magnesium Carbonat	84.31420	-1111.69		±8.	76.262	65.863		†
MgCl	59.75770	-43.51		±42.	34.858	233.423		†
MgCl+	59.75715	652.7		±84.	35.476	228.566		
MgClF	78.75610	-569.02		±21.	49.912	265.994		
MgCl2 (S)	95.21040	-641.62		±0.46	71.509	89.660		†
MgCl2(L)	95.21040	-601.58			---	---		†
MgCl2	95.21040	-392.46		±2.1	57.146	277.041		†
MgF	43.30340	-236.81		±8.4	32.570	221.089		†
MgF+	43.30285	512.29		±46.	32.644	215.348		
MgF2(S)	62.301810	-1124.2		±1.3	61.546	57.243		†
MgF2(L)	62.301810	-1072.35			---	---		†
MgF2	62.301810	-726.76		±16.7	48.264	256.514		†
MgF2+	62.30126	592.		±20.9	52.459	258.152		
MgH	25.31294	169.03			29.557	193.199		†
MgI	151.20947	24.61		±41.8	36.816	252.650		†
MgI2(S)	278,11394	-366.94		±6.3	74.907	129.698		†
MgI2(L)	278.11394	-342.25			---	---		†
MgI2	278.11394	-160.25		±10.5	59.631	317.496		†
MgN	38.31174	288.70	289.04	±25.1	32.761	224.845		†
MgO(S)	40.30440	-601.24		±0.63	37.146	36.938		†
MgO(L)	40.30440	-532.61			---	---		†
MgO	40.30440	58.16		±25.1	32.241	213.299		†
MgOH	41.31234	58.16		±37.7	43.049	226.467		†
MgOH+	41.31179	584.42		±62.8	43.229	220.834		

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
Mg(OH)2(S)	58.31968	-924.66		±2.1	77.264	63.236		†
Mg(OH)2	58.31968	-572.37		±33.5	69.505	267.295		†
MgS(S)	56.37100	-345.72		±4.2	45.605	50.329		†
MgS	56.37100	-145.23		±66.9	34.664	225.518		†
MgSO4(S)	120.36860	-1261.79		±20.9	96.209	91.393		†
MgSO4(L)	120.36860	-1246.59			---	---		†
MgSiO3 (S)	100.38870	-1548.92		±4.2	82.198	67.839		†
MgSiO3 (L)	100.38870	-1494.86		±20.9	---	---		†
MgTiO3(S)	120.18320	-1572.56		±6.3	91.953	74.583		†
MgTiO3(L)	120.18320	-1497.63		±6.3	---	---		†
MgTi2O5(S)	200.06200	-2509.36		±10.5	147.009	135.655		†
MgTi2O5 (L)	200.06200	-2382.31		±8.4	---	---		†
Mg2	48.61000	287.63		±08	24.293	240.189		†
Mg2F4	124.60361	-1718.37		±37.7	107.553	337.041		†
Mg2SiO4(S)	140.69310	-2176.94		±4.2	119.151	95.239		†
Mg2SiO4(L)	140.69310	-2113.88		±20.9	---	---		†
Mg2TiO4(S)	160.48760	-2164.38		±6.3	128.724	115.153		†
Mg2TiO4(L)	160.48760	-2046.33			---	---		†
MnO (S)	70.93745	-385.221			44.102	59.71		
MnO2(S)	86.93685	-520.029			54.415	53.049		
Mn2O3 (S)	157.8743	-959.002			99.034	110.499		
Mn3O4 Solid-A	228.81175	-1387.799			140.515	155.599		
Mn5N2(S)	302.70373	-204.2			175.724	187.443		
MnS Solid	87.00405	-214.2			49.943	78.199		
MnS2 (S)	119.07005	-223.844			70.075	99.914		
Mo(cr) REFERENCE ELEMENT	95.94	0	0		23.933	28.605		*‡
MoC Solid-C	107.951	-28.451			30.878	36.652		
MoO2 Solid	127.9388	-588.94			55.982	46.275		
MoO2	127.9388	-8.314			34.002	252.344		
Mo2C(S)	203.891	-53.137			60.207	65.814		
N	14.00674	472.68		±0.4	20.786	153.302		†
ND	16.0208	355.309	355.710	±8.	29.159	187.234	8.648	†
NHD Radical	17.028782	178.165	181.106	±8.	33.703	205.600	9.912	#
ND2	18.0349	181.937	184.878	±8.	34.415	204.335	9.962	†
ND2H	19.04288	-52.748	-45.684		35.976	209.279	10.074	#
ND3	20.04901	-54.501	-47.546	±0.4	38.225	203.931	10.234	†#
NF	33.00514	232.99	233.	±3.	30.228	212.908	8.738	†
NF2	52.00355	34.421	37.000	±5.	41.058	249.638	10.582	†
NF3	71.00195	-131.7	-125.98	±1.	53.497	260.812	11.855	†
NH	15.01468	358.792	358.76	±0.37	29.193	181.227	8.601	†
NH+	15.01413	1665.795	1656.29		32.775	187.651	9.495	†
NHF	34.01308	112.0	114.952	±15	35.234	230.806	10.030	†
NHF2	53.01149	-103	−96.413	±15	43.384	252.814	10.807	†
NH2 AMIDOGEN RADICAL	16.02258	186.2	189.1	±1.0	33.663	194.868	9.911	#
NH2D	18.03672	-48.697	-41.627		35.157	205.591	10.018	#
NH2F	35.02102	-75	-67.889	±15.	36.474	229.534	10.105	†
NH3 AMONIA RRHO calc	17.03056	-45.567	-38.513	±0.03	34.597	192.475	9.984	#
NH3 AMONIA Anharmonic calc	17.03056	-45.567	-38.946	±0.03	35.630	192.770	10.043	†
NH2OH Hydroxyl Amine	33.02996	-43.95	-33.809	±0.55	46.472	236.181	11.236	†#
NH4+ AMONIUM ION	18.03795	644.905	637.358	±0.37	34.764	186.095	9.987	†
NH4CLO4(I)	117.4888	-295.767	-277.78		128.072	184.18	25.238	†
NO	30.00614	91.271	90.767		29.862	210.748	9.179	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
NO+	30.00559	990.807	982.137	±60.	29.123	198.234	8.670	†
NOCL	65.45884	52.524	54.425	±0.5	44.623	261.590	11.364	†
NOF	49.00454	-65	-62.633	±2.0	41.530	248.224	10.720	†
NOF3	87.00135	-187	-178.78	±7.	68.067	277.731	13.698	†
NO2	46.00554	34.193	37.0	±0.5	37.177	240.171	10.208	†
NO2-	46.00609	-191.518	-182.482	±0.47	37.215	236.241	10.177	†
NO2CL	81.45824	12.5	17.901	±1.	53.246	272.128	12.205	†
NO2F	65.00394	-109	-102.92	±20	48.999	259.287	11.347	†
NO3	62.00494	74.628	81.024	±0.69	46.935	252.623	10.959	†
NO3-	62.00549	-312.185	-299.405	±0.65	44.724	245.638	10.733	†#
NO3F	81.00334	15			66.958	293.171		†
N2 REFERENCE ELEMENT	28.01348	0	0		29.124	191.607	8.670	‡†
N2D2 Cis	32.0416	202.857	209.788		39.025	224.095	10.308	†#
N2F2	66.01029	62.374	67.	±10	56.569	268.216	12.869	†
N2F4	104.00709	-22	-13.491	±10	88.384	317.531	17.812	†
N2H	29.02142	251.776	254.707	±8.	34.662	224.507	9.973	#
N2H2	30.02936	211.859.	219.	±10	35.045	218.333	9.997	†
NH2NO2 NITRAMIDE	62.02816	-26.000	-12.346	±10	56.672	268.548	12.164	†
H3N2 HYDRAZINE RAD	31.0373	220.659	209.946	±8.	34.358	236.791	10.634	#
N2H4(L) Hydrazin	32.04524	50.38	--		98.839	121.545	--	†
N2H4 HYDRAZIN	32.04524	95.18	109.337	±0.5	48.43	238.466	11.449	†
NH4NO3 (solid)	80.04344	-365.6	--	±1	139.080	150.810	--	†
N2O (NNO)	44.01288	81.6(82.6)	85.029	±0.1	38.628	220.01	9.581	†
N2O+	44.01233	1333.399	1329.146	±0.63	42.263	233.859	10.623	†
N2O3	76.01168	86.631	91.2		72.733	314.736		†
N2O4	92.01108	11.111	20.4	±0.14	79.168	304.451	16.741	†#
N2O5	108.01048	15.437	25.010	±0.74	95.332	355.717	20.797	†#
N3 AZIDE RADICAL	42.02022	453.54	456.97	±3.5	36.175	223.072	9.571	†#
N3H (s) Azidic Acid	43.02816	261.59		±0.77				X
N3H AZIDIC ACID	43.02816	291.713	298.005	±0.65	44.219	239.330	10.947	†#
N4H4 NH4N3 (cr)		114.14		±0.94				X
N4H4 NH4N3 (g) ??		179.7 ?	doubtful	exis-	tence			X
Na(cr) REFERENCE ELEMENT	22.98977	0	0		28.230	51.300	6.460	†
Na(g)	22.98977	107.5	107.763	±0.7	20.786	153.719	6.197	†
Na+	22.98922	609.34	--		20.785	147.953	6.197	†
NaO2(cr)	54.98857	-261.	-264.16	±3.	72.130	115.900	18.300	†
Na2O(cr)	61.97894	-417.98	(-413.15)	±4.2	69.103	75.042	12.399	*†
Na2O(liq)	61.97894	-372.843	--		104.600	91.607	--	†
Na2O (g)	61.97894	-16.56	-13.710	±10.	56.773	271.324	14.410	†
Na2O2(cr)	77.97834	-513.21	(-507.34)	±5.	89.266	94.801	15.707	*†
Na2O2(g)	77.97834	-123.93	-117.895	±30.	68.503	289.595	15.565	†
Ne REFERENCE ELEMENT	20.1797	0	0		20.786	146.33	6.197	*‡
Ne+	20.17915	2086.966	2080.66	±0.001	22.120	158.310	6.304	†
Ni(cr) REFERENCE ELEMENT	58.6934	0	0		25.987	29.87	4.786	*‡
NiO Solid-A	74.689	-8.314			44.309	37.991		
NiS(b) Crystal	90.7594	-87.869		±6.3	47.121	52.986		*
NiS2(s)	122.8254	-131.381		±16.7	70.627	71.966		*
Ni3S2(l)	240.2122	-216.325		±5	117.75	133.871		*
Ni3S4(s)	304.3442	-301.121		±25.1	164.813	186.484		*
O	15.99940	249.175	246.79	±0.1	21.912	161.06	6.725	†
O singlet (excited)	15.99940	458.523	436.666		20.786	156.816	6.197	#
O-	15.99995	101.846	105.813		21.685	157.797	6.571	†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
O2 REFERENCE ELEMENT	31.99880	0	0		29.378	205.149	8.680	*‡
O2 singlet (excited)	31.99880	94.418	94.409		29.485	201.915	8.689	#
O2+	31.99825	1171.828	1165.		30.67	205.393	9.311	†
O2-	31.99935	-48.028	-42.5		31.422	209.336	9.350	†
O3 OZONE	47.9982	141.8	144.454		39.378	239.011	10.366	†
P	30.97376	316.39		±1	20.786	163.2		†
PCL3	137.33186	-288.58		±5.4	71.706	311.715		*†
PF	49.97217	-52.377		±20.9	31.616	224.968		*†
PF2	68.97057	-488.269		±20.9	44.716	262.958		*†
PF3	87.96897	-958.457		±3.8	58.801	273.073		*†
PF5	125.96578	-1594.433		±2.9	85.05	300.855		*†
PH	31.9817	230.752	231.698	±33.5	29.175	196.381	8.648	†
PH2 Phosphonium Radical	32.989641	135.474	139.333	±8.	34.272	212.710	9.969	#†
PH2-	32.990190	-9.265	+0.800	±10.	34.124	205.247	9.960	†
PH3 PHOSPHINE RRHO	33.997581	11.786	19.712	±8.	37.102	210.245	10.137	#†
PN	44.9805	104.776			29.667	211.126		*
PO	46.97316	-29.597		±4.2	31.725	222.768		*
PO2	62.97256	-314.533			41.397	253.682		*
P2	61.94752	143.651		±2.1	32.057	218.135		*
P4	123.89505	58.917		±2.1	67.326	280.022		*
P4O6	219.89145	-2144.519		±33.5	143.998	345.664		*
P4O10(s)	283.88905	-3010.022		±8.9	211.82	228.786		*
P4O10	283.88905	-2904.154		±8.9	188.827	403.974		*
Pb (cr) REFERENCE RLEMENT	207.2	0.	0.		24.430	36.899	6.870	†
Pb (gas)	207.2	195.2	195.88	±0.8	20.786	175.377		†
PbBr	287.1040	64.821	73.805	±20	36.916	272.744	10.146	†
PbBr2	367.0080	-103.908	-87.54	±7.	56.966	339.673	15.022	†
PbBr3	446.9120	-104.011	-80.330	±80.	80.540	385.255	19.969	†
PbBr4	526.8260	-182.436	-152.4	±80.	104.468	427.724	25.871	†
PbCl	242.65270	8.819	10.493	±12.	36.215	261.306	9.787	†
PbCl2	278.10540	-175.046	-173.5	±5.	55.299	315.621	14.003	†
PbCl3	313.55810	-177.654	-175.27	±80.	77.918	351.604	18.256	†
PbCl4	349.0108	-327.43	-325.65	±80.	100.537	381.682	23.449	†
PbF	226.19840	-98.072	-96.853	±10.	34.401	249.962	9.268	†
PbF2	245.19681	-443.427	-440.30	±11.	50.981	291.532	12.573	†
PbF3	264.19521	-489.573	-485.0	±60.	70.582	316.287	15.535	†
PbF4	283.1936	-799.925	-795.03	±60.	90.232	331.825	19.626	†
PbI	344.10447	108.904	112.033	±4.	37.152	280.413	10.339	†
PbI2	461.00894	-10.253	-5434	±5.	57.182	352.613	15.247	†
PbI3	587.91341	21.755	27.35	±80.	81.624	411.532	21.065	†
PbI4	714.81788	-41.281	-35.485	±80.	106.276	463.806	27.521	†
PbO(S)	223.19940	-218.6	-216.61	±0.5	46.414	67.840	9.225	†
PbO	223.19940	68.187	70.385	±4.5	32.513	240.045	8.962	†
PbO2(S)	239.19880	-276.0	-271.41	±1.5	60.997	71.920	10.962	†
PbO2	239.19880	136.153	139.452	±100.	51.721	261.093	12.251	†
PbS(S)	239.2660	-99.475	-99.703	±	49.499	91.200	11.510	†
PbS	239.2660	127.945	129.797	±1.5	35.085	251.414	9.430	†
PbS2	271.3320	244.049	245.722	±10.	57.511	286.141	14.021	†
PbN6(S) Lead Azide	291.3	469.						X
S(S) REFERENCE ELEMENT	32.066	0	0		22.690	33.070	4.412	‡†
S	32.066	277.17	274.925	±0.25	23.674	167.832	6.657	†
SCL	67.5187	156.47		±16.7	37.555	237.334		*†

Table 6 (continued)

Compound	Mol. Wgt.	$\Delta_f H_{298}$ kJ/mol	$\Delta_f H_0$ kJ/mol	± kJ/mol	C_{p298} J/mol/K	S_{298} J/mol/K	H_{298}-H_0 kJ/mol	
SCL2	102.9714	-17.572		±3.3	50.909	281.641		*†
SF	51.0644	12.971		±6.3	35.157	225.282		*†
SF2	70.06281	-296.653		±16.7	44.906	257.708		*†
SF3	89.06121	-503.041		±33.5	62.998	286.186		*†
SF4	108.05961	-763.18		±20.9	77.62	299.657		*†
SF5	127.05802	-908.467		±15.1	89.687	304.774		*†
SF5Br	206.96202	-972.8		±59	107.075	333.654		
SF5CL	162.51072	-1038.9		±10.5	104.344	319.936		
SF6	146.05642	-1220.502		±0.8	96.994	291.551		*†
SN	46.07274	263.583		±105	31.758	222.081		*
SO	48.0654	5.008		±1.3	30.164	221.944		*
SOF2	86.06221	-543.926		±105	57.202	279.156		*
SO2	64.0648	-296.835		±0.21	39.867	248.206		*
SO2CLF	118.5159	-556.476		±21	71.719	302.879		*
SO2CL2	134.9702	-354.802		±2.1	77.218	311.127		*
SO2F2	102.06161	-758.569		±8.4	65.946	283.651		*
SO3	80.0642	-395.753		±0.71	50.692	256.775		*
S2	64.132	128.404		±.0.3	32.481	228.313		*
S2CL	99.5847	78.562		±8.4	50.968	292.162		*
S2CL2	135.0374	-16.736			72.776	327.237		
S2F2 (SSF2)	102.11681	-401.422		±41.8	63.146	292.729		*
FS2F	102.11681	-336.443		±41.6	66.061	293.985		*
S2F10	254.11603	-2064.386		±29.3	176.702	397.041		
S2O	80.1314	-56.486		±33.5	44.112	267.029		*
S8	256.528	100.42		±0.63	156.046	430.319		
Si(cr) REFERENCE ELEMENT	28.0855	0	0		19.789	18.81		*‡
SiC(b)	40.0965	-73.22			26.867	16.617		*
SIF2 DifluoroSilylene	66.082306	-627.014	-626.2	±16.8	44.707	256.710	11.228	#
SiF3 TrifluoroSilyl Radical	85.080710	-993.365	-990.4	± 8.	59.613	282.433	13.398	#
SiF4 TetrafluoroSilane	104.07911	-1614.98	-1609.4	± 4.2	73.534	282.615	15.325	#
SiHF3 TriFluoroSilane	86.088650	-1207.67	-1200.5	± 5.4	63.486	277.351	13.545	#
SiO2(Lqz) Quarz	60.0843	-910.857			44.59	41.463		
Si2N2O(s) Silicon Oxynitride	100.18388	-947.711			67.46	46.06		
Si3N4(a) Silicon Nitride	140.28346	-744.77			99.579	112.968		*
SiS2 Solid	92.2175	-213.384			77.482	80.333		#
SnCl4 TetraChloroStanum	260.52080	-478.650	-476.30	±4.2	98.459	364.549	22.340	†#
SnH3 TriHydroStanum Radical	121.73382	258.153	266.252	±4.2	44.818	240.204	10.926	#
SnH4 TetraHydroStanum	122.74176	162.758	174.594	±4.2	51.108	228.991	11.423	#
Xe REFERENCE ELEMENT	131.29	0	0		20.786	169.686	6.197	*‡
Xe+	131.28945	1176.552	1170.35		20.786	181.212	6.197	†
Zn(cr) REFERENCE ELEMENT	65.39	0	0		25.390	41.630	5.657	‡
ZnCL2	136.29540	-265.684	-		56.902	276.672	-	
ZnSO4 (cr)	161.4536	-980.144	-969.95	± 4.2	99.035	110.541	17.238	†

* The polynomials are pinned at 1000 K, therefore the property values are not exact at 298 K. All other polynomials are pinned at 298 K, therefore the property values are exact.

\# 9 term NASA polynomials are available in the NEWNASA.TXT file for this species.

† 9-term NASA polynomials are available in http://cea.grc.nasa.gov

Table 6 (continued)

‡ 9-term NASA polynomials for all Reference Elements are available in the ELEMENTS.DAT file.
X Polynomials not available